Naval Research Laboratory

Washington, DC 20375-5320

NRL/MR/6003--19-9855

Highly Complex Fluid Dynamics: NRL 6.1 Work Unit 4464 Closeout Report

Jay Boris

Laboratories for Computational Physics and Fluid Dynamics Branch
Material Science & Component Technology Directorate

February 7, 2019

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
07-02-2019

2. REPORT TYPE
Memorandum Report

3. DATES COVERED *(From - To)*

4. TITLE AND SUBTITLE
Highly Complex Fluid Dynamics: NRL 6.1 Work Unit 4464 Closeout Report

5a. CONTRACT NUMBER

5b. GRANT NUMBER
64-1G56-0-9-5

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Jay Boris

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
U.S. Naval Research Laboratory
4555 Overlook Avenue, SW
Washington, DC 20375-5320

8. PERFORMING ORGANIZATION REPORT NUMBER
NRL/MR/6003--19-9855

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSOR / MONITOR'S ACRONYM(S)

11. SPONSOR / MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT
DISTRIBUTION STATEMENT A: Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
Work Unit 4464 in the Computational Physics Task Area was entitled "Highly Complex Fluid Dynamics." It ran from 2011 to 2018 at about the one manyear, senior scientist, level. Work here leveraged and was leveraged by our multi-year CRADA collaboration with the environmental wind tunnel team at the University of Hamburg, Germany. NRL participants, beyond the Principal Investigator, included Gopal Patnaik, Adam Moses, and Keith Obenschain of Code 6040. This closeout report is an annotated bibliography with commentary, of the 32 papers, reports, and articles produced during this 6.1 basic research program. The nine papers, reports and drafts describing new innovations, research results and capabilities from the work unit that seem most important, are briefly summarized at the end in Section III. Presentations have generally been excluded from this annotated bibliography in the interests of brevity.

15. SUBJECT TERMS
Highly Complex Fluid Dynamics
Plume Model Health Effects
Urban Weapons of Mass Destruction
Airborne Contaminant Transport
Large Eddy Simulation Non-Equilibrium Turbulenece

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
Unclassified Unlimited	Unclassified Unlimited	Unclassified Unlimited	Unclassified Unlimited	25	Jay Boris
					19b. TELEPHONE NUMBER *(include area code)* 202-767-3055

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

This page intentionally left blank.

Highly Complex Fluid Dynamics:
NRL 6.1 Work Unit 4464 Closeout Report

Dr. Jay Boris, Principal Investigator, Code 6003

Abstract:

Work Unit 4464 in the Computational Physics Task Area was entitled "Highly Complex Fluid Dynamics." It ran from 2011 to 2018 at about the one manyear, senior scientist, level. Work here leveraged and was leveraged by our multi-year CRADA collaboration with the environmental wind tunnel team at the University of Hamburg, Germany. NRL participants, beyond the Principal Investigator, included Gopal Patnaik, Adam Moses, and Keith Obenschain of Code 6040. This closeout report is an annotated bibliography with commentary, of the 32 papers, reports, and articles produced during this 6.1 basic research program. The nine papers, reports and drafts describing new innovations, research results and capabilities from the work unit that seem most important, are briefly summarized at the end in Section III. Presentations have generally been excluded from this annotated bibliography in the interests of brevity.

I. Objectives: The original objectives were:

A. New Capabilities: Provide new multi-physics algorithms, demonstrated in working Computational Physics models, that significantly extend the validity and efficiency of current state-of-the-art Computational Fluid Dynamics capabilities to enable accurate computation of complex fluid dynamics. B. Demonstration Problems and Applications: 1) Provide fast computational realizations of fine grain turbulence to be used as "ground truth" for UAV flight dynamics research, 2) Provide fluctuating boundary conditions to improve the accuracy of FAST3D-CT simulations, 3) Provide quantitative understanding of particle/droplet deposition on surfaces and bubble rise and dispersion that can be used to develop and calibrate fast models, 4) Provide a fast Large Eddy Simulation (LES) model of a ship's wake and bubble dispersion, and 5) Demonstrate a fast algorithm to couple the models from 1) and 3) to represent flow and deposition inside a complex tunnel system (contaminant transport) and in a complex micro-channel configuration. C. Impact: The results of topics 1, 2 and 4 will improve environmental estimates of in situ tracer plumes for testing and evaluating proposed sensors for IED applications. This research will also establish a needed baseline capability for future Autonomous Systems Laboratory scenarios involving swarms of UAVs or other airborne autonomous systems. Much of the research proposed here is high risk in the sense that the desired accuracy or performance goals may not be met easily.

Comments: At the Triannual External Review of the Computational Physics Task Area in 2018, results in the following topics were presented and discussed:

- Synthetic Turbulence, and Fluctuations in Turbulence and Reactive Flow

* Coherent Structure Dynamics: Model for Non-Equilibrium Turbulence

* Blending Different Resolution CFD Solutions

- Remediation of Airborne Contaminants in Flight

Manuscript approved February 7, 2019.

* Proximity Analysis for Model Calibration and Validation

* Approach for Computing Fast Radioactive Cloud Shine

The topics marked with asterisks will probably turn out to be the most important contributions. These and other results are briefly described in terms of the reports, software documentation, and papers produced from participants in the work unit. These efforts are presented in roughly chronological order below. The particle droplet-bubbly wake objective never took flight in this work unit as a project. It was undertaken in conjunction with Code 7100 (Steve Stanic) by Russell Dahlburg. Further, Drs. Kailasanath and Schwer conducted ground-breaking research at about the same time on sectional representation of multiphase flows with important particle components in Dr. Kailasanath's 6.1 work units.

The objective about flow in channels (micro-channels and tunnels) was proposed to leverage planned efforts in computing the flow of air and blood in the human body ("The Computational Man") and in tunnel systems such as subways and terrorist emplacements. These efforts were predicated on leveraging applications for DTRA (former) and DHS (latter) that never actually materialized.

Computing Fast Radioactive Cloud Shine was researched at the beginning of the program to provide a requested augmentation for NRL's evolving, real time airborne contaminant prediction system, CT-Analyst®. Several cities, including Los Angeles, then a collaborator on a funded DHS project installing sensors and a real-time system based on CT-Analyst, requested the capability for computing radioactive cloud shine based on their concern about nuclear and dirty bomb threats to L.A. Radioactive clouds are a potential threat, even beyond the area where the cloud can be inhaled, because the radioactivity 'shines' beyond the extent of the cloud presenting a threat some distance beyond the radioactivity. The computation from first principles is very slow so existing software (DOE) takes some minutes to execute and is not very flexible with respect to supporting time-critical applications in complex geometry.

Early in this work unit, several months of effort were undertaken to breadboard a new approach that changed the method of representing the 3D geometry of the city by pre-processing the slow portions and by restructuring the 4D integral over the evolving cloud density. A meaningful demonstration calculation was conducted in breadboard form using the fictitious city geometry of 29 Palms. The calculation took several seconds and could have been eventually engineered to run that fast in CT-Analyst. It was shown in a number of DHS venues and opportunities but support never became available. Other research activities and publication efforts eventually took priority.

II. Reports, Papers, and Publications:

The How and Why of Nomografs™ for CT-Analyst®, J. Boris, G. Patnaik., K. Obenschain, NRL/MR/6440–11–9326, May 2011.

ABSTRACT: An urban-oriented emergency assessment system, called CT-Analyst®, was developed to evaluate airborne contaminant transport (CT) threats and aid rapid decisions for regions such as cities where other methods are slow and inaccurate. CT-Analyst gives both greater accuracy and much greater speed than alternate prediction tools because it embodies entirely new principles to function in the information-starved situations that characterize the first few minutes of a terrorist or accident scenario. CT-Analyst was designed for the military prior to 9/11 to use verbal and sensor reports, to use mobile sensors, and to function in realistic situations, such as the first few minutes of a harbor spill, where information about the airborne contaminant or chemical, biological, radiological (CBR) agent is highly uncertain. These improvements are made possible by pre-computing very accurate three-dimensional flow solutions that include solar heating, buoyancy, complete building geometry, trees, and impressed wind fluctuations. Detailed 3D simulations for 18 wind directions are pre-computed for coverage regions where CT-Analyst is to be installed. CT-Analyst extends these results to all wind directions, speeds, sources, and source locations through a new data structure called Dispersion NomografsTM. We generate these "nomografs" for cities, ports, and industrial complexes well in advance so a manager in an emergency need not wait for supporting analyses. CT-Analyst also provides new real-time functions such as sensor data fusion, "backtracking" reports and observations to an unknown source location, and even evacuation route planning. The resulting capability is faster, more accurate, more flexible, and easier to use than Gaussian and particle-based dispersion models.

Comment: Our German colleagues and sponsors requested this report be written to explain the underpinnings of the CT-Analyst data representation that allows all the plume shapes for a rectangular domain some kilometers in extent and for a given wind direction to be reduced to a few megabytes of data in a 2D array.

High-Fidelity Plume Model Health Effects and Integrated Simulation and Training Tools, A. Moses, J. Boris, G. Patnaik & K. Obenschain, also Proceedings: 15th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, 12–14 July 2011.

Comment: This was a conference presentation with a slide deck available in the proceedings. CT-Analyst® was integrated into the Army/Marine virtual battlefield simulator VBS2 so virtual training could be performed with realistic real-time agent plume modes provided by an integrated CT-Analyst system. Although this activity did not go much further at this time, it represents a potentially important contribution to the military and civilian training communities.

Validating the LES-Based Emergency Response Tool CT-Analyst for Use in a European City, F. Harms, D. Hertwig, B. Leitl, M. Schatzmann, G. Patnaik, M-Y. Obenschain, J. Boris, and K. Obenschain, Proceedings: 15th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, 12–14 July 2011.

Comment: This was a conference presentation with a slide deck available in the proceedings. The paper reports the experimental field trials conducted in Hamburg Germany testing NRL's CT-Analyst operational WMD prediction tool, which is now in 24/7 use.

LES validation for turbulent flow in an urban environment, Denise Hertwig, Frank Harms, Bernd Leitl, Gopal Patnaik, Mi Young Obenschain, David Fyfe, Proceedings: 15th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, 12–14 July 2011.

Comment: This was a conference presentation with a slide deck available in the proceedings. The paper reports the comparison of NRL's FAST3D-CT Large Eddy Simulation code and detailed wind tunnel studies conducted at Hamburg University. These three proceedings papers reported work at the main US Atmospheric Transport and Modelling Conference by the collaboration between NRL and Hamburg which was initiated by DTRA, NRL, and ONR Global and grew into a multi-year CRADA supporting the joint efforts.

An LES-Based Microscale Airborne Hazard Model, M. Schatzmann, B. Leitl, D. Hertwig, F. Harms, C. Peeck, G. Patnaik, J. Boris, K. Obenschain, S. Fischer and P. Rechenbach, Proceedings: 14th International Conference on Harmonization within Atmospheric Dispersion Modeling for Regulatory Purposes, Kos Island, Greece, 2–6 October 2011.

Abstract: First responders need a more or less instant estimate of danger zones resulting from accidentally released hazardous materials in order to take immediate action, to coordinate rescue teams and to protect human population and critical infrastructure. To fulfil the need for a sufficient dispersion modelling accuracy while maintaining efficient access to reliable results in a first responder's environment, high-resolution, pre-incident LES modelling can be combined with 'physical data reduction' in an emergency assessment tool. A typical example of such an approach adjusted to the geometry of the Hamburg inner city area will be presented.

Manufacturing, storing and transportation of flammable and toxic gases involves the risk of accidental spills of hazardous materials. Releases of major concern occur in urban or industrial environments, with the consequence that the dispersion is heavily influenced by buildings and other obstructions. Dispersion models of different complexity have been developed in the past. Although they have been reasonably successful in some cases, most of them are still limited in scope. Especially in cases where obstacle effects dominate the dispersion of the hazardous cloud, these models are either too simplistic and thus unable to cope with the geometric complexity, or they are much too slow and thus not able to provide immediate guidance for the persons in charge of the rescue operations.

Recent progress in the fields of computer hardware development, numerical mathematics and scientific computing opens up the potential for improvements. In an effort jointly carried out by the Ministry of the Interior of the Free and Hanseatic City of Hamburg, by the US Naval Research Laboratory and by the Meteorological Institute of the University of Hamburg, a new emergency management tool for the Hamburg inner city area has been developed. This tool provides, nearly instantaneously, the space-time-structure of airborne hazardous clouds. It is based on a high- resolution LES contaminant transport model (FAST3D-CT) which provides the detailed velocity and turbulence fields within the urban domain. This database is then converted to an efficient form suitable for use in a second model (CT-Analyst) which runs on a laptop and comes with an interface as is common in computer games. The system is fast because results are pre-computed for a large number of meteorological situations. In case of an accident predictions are based solely on already existing knowledge. The system is easy to handle due to its user-friendly interface. Subsequently details of the new emergency management tool for the city of Hamburg will be presented.

LES Validation of Flow in a Densely Built Environment, Denise Hertwig, Christine Peeck, Frank Harms, Gopal Patnaik, Bernd Leitl, And Michael Schatzmann, Proceedings: 14th

International Conference on Harmonization within Atmospheric Dispersion Modeling for Regulatory Purposes, Kos Island, Greece, 2–6 October 2011.

Abstract: In a systematic study wind-tunnel measurements and predictions from large-eddy simulation (LES) of turbulent flow in the inner city of Hamburg, Germany, are compared. The reference laboratory measurements of velocity fields are carried out in a neutrally stratified boundary-layer wind tunnel within an urban model on a scale of 1:350. Numerical results are obtained from simulations with the implicit LES code FAST3D-CT. The numerical model is developed and operated by the U.S. Naval Research Laboratory and is based on a monotone integrated large-eddy simulation (MILES) methodology. The focus of the validation exercise is the comparison of time-series information and the characterization of turbulent flow structures within and above the urban canopy. On the basis of densely spaced measurements in vertical profiles and horizontal flow layers the developments of the turbulent boundary-layer within the city as well as typical street-canyon flow scenarios provide the framework for this analysis. Particular challenges with respect to the validation of time-resolved simulations in contrast to standard approaches are discussed with an emphasis on specific demands in the case of urban flow fields.

Characterization of Transient Dispersion Processes in an Urban Environment, F. Harms, D. Hertwig, B. Leitl, M. Schatzmann, G. Patnaik, Proceedings: 14th International Conference on Harmonization within Atmospheric Dispersion Modeling for Regulatory Purposes, Kos Island, Greece, 2–6 October 2011.

Abstract: Validating LES-based flow and dispersion models for the purpose of predicting transient flow and dispersion phenomena is more demanding than validating RANS-based codes. Since the model output is no longer related to stationary or quasi-stationary boundary conditions, and since the model results are not restricted to mean flow and average dispersion patterns, an evaluation of the model based on mean results is no longer adequate. A more sophisticated but also more complex validation approach based on statistically representative ensembles is required. Reference data is needed which reliably identifies mean as well as extreme values of concentration, dosage and cloud travel times for a given dispersion scenario. An example of how systematic wind tunnel measurements can characterize transient dispersion processes of puffs in a complex urban environment is given.

Comments: These three papers directly above, published in a conference proceedings volume, record some of the first efforts funded jointly by the work unit and the CRADA collaboration with Hamburg. Hamburg university academics from their environmental wind tunnel team, led by Professor Leitl, and the city officials, led by Dr. Suzanne Fischer, became major proponents for CT-Analyst and the validation activities surrounding it as CT-Analyst became Hamburg's primary 24/7 atmospheric incident system.

Mit CT-Analyst im Störfalleinsatz "vor die Lage Kommen," Susanne Fischer, Peer Rechenbach, Knut Storm, Michael Schatzmann, Bernd Leitl, Denise Hertwig, Frank Harms, Gopal Patnaik, and Jay Boris, *Bevolkerungsschutz of the German Federal Office of Civil Protection and Disaster Assistance*, pg. 12–19, April 2012.

Abstract: Meteorologen der Universität Hamburg, Strömungswissenschaftler der US-Marine und Praktiker der Hamburger Sicherheitsbehörden haben in einem gemeinsamen zweijährigen Projekt eine neuartige Software für den Einsatz bei Schadstoffunfällen entwickelt. CT-Analyst bietet u.a. die Möglichkeit, Schadstoffausbreitungen, etwa nach Industrieunfällen oder terroristischen Anschlägen, zu prognostizieren, mögli- che Gefahrenbereiche anzuzeigen, aber auch im Einsatz einen noch unbekannten Freisetzungsort zu lokalisieren. Das Projekt wurde vom BBK und der Hamburgischen Bürgerschaft finanziell gefördert.

Meteorologists from the University of Hamburg, US Navy scientists and practitioners from the Hamburg safety authorities have developed novel software for use in pollutant accidents in a joint two-year project. CT analyst offers the possibility of predicting the spread of pollutants, for example after industrial accidents or terrorist attacks, to indicate possible danger areas, but also to localize a still unknown release site during operation. The project was financially supported by the BBK and the Hamburgische Bürgerschaft.

Comment: Our German colleagues regularly have to describe their work (often our joint work) to their local authorities and hazmat people. The result is occasional papers such as this written for trade journals and other government publications in Germany.

Effect of Nozzle-Exit Flow Conditions on the Flow and Acoustic Properties of Imperfectly Expanded Supersonic Jets, J. Liu, K. Kailasanath, J.P. Boris, N. Heeb, D. Munday, and E. Gutmark, AIAA 2012–2161, 18 AIAA/Confederation of European Aerospace Societies (CEAS), Colorado Springs CL, 4–6 June, 2012, (AIAA, Reston VA, 2012).

Abstract: The impact of the turbulence level at the nozzle exit on the jet flow and far-field noise level has been investigated using large-eddy simulations (LES) and the Ffowcs Williams & Hawkings (FW-H) surface integral method. The jet exit flow condition is slightly under- expanded. Both the random perturbations inside the nozzle and the nozzle surface roughness are used to increase the turbulence level. Increasing the turbulence level at the nozzle exit increases the shear-layer spreading, reduces the screech intensity and also decreases slightly the far-field noise level. The LES predictions of the shock-cell structures and the jet core lengths agree well with the measurement data. In addition, the impact of grid resolution used in both the jet flow and the near-field acoustic propagation region has also been investigated. It is found that the grid resolution used in the shear layer impacts the numerical predictions more than those used in the other regions. Adding an adequate amount of turbulence level at the nozzle exit greatly improves the predictions using a coarser grid resolution in the shear layer. Furthermore, the far-field noise predictions agree well with measurement data, and the contribution from the end cap is found small, but it is sensitive to the mesh size used in the integration.

Comment: One of the earliest "turbulence" problems tackled in the work unit was to find a way to approximate a time-dependent, non-periodic "turbulent" perturbation of the flow near a wall in the JENRE calculations of noise generation in a military jet exhaust. A simple, easy-to-evaluate formula was developed that could be scaled and which would have a wide spectrum of perturbations to allow coarser grid resolution of the shear layer without having to resolved the actual boundary layer turbulence. Jun Liu has recently found an improved method that allows approximating the effect of a turbulent boundary layer over a larger area. During this work, a method was found to define a set of smooth basis functions each of which had a

Kolmogorov spectrum, and interesting oddity still awaiting an application. This research had an important short-term impact but is unlikely to have major lasting value.

Effect of the Initial Turbulence Level on an Underexpanded Supersonic Jet, J. Liu, K. Kailasanath, J.P. Boris, N. Heeb, D. Munday, and E. Gutmark, *AIAA Journal 51* (3), 741–745, March 2013.

Abstract: NOZZLE exit conditions in jet flows may impact shear-layer spreading, jet core length, peak turbulence level, and associated noise generation [1–4]. Among the variables that define the nozzle exit conditions the initial turbulence level was found to have a dramatic effect in subsonic jet flows and may have been the primary reason for the scatter in the measurement data reported in [2]. Bogey and Bailly [4] also reported a large impact of the initial turbulence level in their subsonic jet flow simulations. They found that increasing the initial turbulence level weakens the coherent vortex pairing, increases the jet core length, and reduces the shear-layer growth rate. On the other hand, in imperfectly expanded supersonic jet flows, it was observed in [3] that increasing the turbulence level at the nozzle exit increases the shear-layer thickness downstream of the nozzle exit, inhibits the formation of the screech tones, and alters the level of shock-associated noise. However, very little work has been reported in quantifying the impact of the initial turbulence levels in large-eddy simulations (LESs) of imperfectly expanded supersonic jet flows.

In this paper, we report on a brief investigation of the impact of the turbulence level at the nozzle exit on the jet flow development and also on the noise characteristics of a slightly underexpanded jet flow using LES. Two approaches of increasing turbulence level at the nozzle exit were employed. The first approach adds random perturbations to the flow field inside the nozzle, and the second approach uses nozzle surface roughness. The advantage of the first approach is its simplicity, and the advantage of the second approach is that the generation of turbulence is a solution of the flow equations. The first approach has been used by several authors in the past [4–8]. For example, random perturbations of the pressure field were used in [5] for simulations of subsonic jets and in [6] for simulations of an over expanded heated jet. In addition, random perturbations of the velocity field with some physical constraints have also been used in simulations of subsonic jet flows [4,7–8]. Because it is easier to change the turbulence level by adjusting the perturbation level inside the nozzle than by adjusting the magnitude of the nozzle surface roughness, the impact of the initial turbulence level was studied primarily through the first approach in which random perturbations with small percentages of the local energy values are added to the energy field. A simulation using the wall roughness was also carried out for comparison.

Comment: This Technical Note expanded on the results of the previous paper (just above) considering surface roughness as well as turbulent fluctuation effects on the sound generated by a supersonic jet exhaust.

Large Eddy Simulation of Accidental Releases, Bernd Leitl, Denise Hertwig, Frank Harms, Michael Schatzmann, Gopal Patnaik, Jay Boris, Keith Obenschain, Susanne Fischer and Peer Rechenbach, in A. Talamelli, M. Oberlack and J. Peinke (Eds.), Progress in Turbulence V, Springer Proceedings in Physics 149, 2013. (University of Hamburg & Ministry of the Interior, Free and Hanseatic City of Hamburg Germany).

Abstract: First responders need a more or less instant estimate of danger zones resulting from accidentally released hazardous materials in order to take immediate action, to coordinate rescue teams and to protect human population and critical infrastructure. To fulfill the need for a sufficient dispersion modeling accuracy while maintaining efficient access to reliable results in a first responder's environment, systematic high-resolution pre-accidental LES modeling can be combined with 'physical data reduction' in an emergency assessment tool. A typical example of such an approach adjusted to the geometry of the Hamburg inner city area will be presented. It gives a glimpse into the application of LES-modeling for real-world problems.

Comment: This publication reviews the FAST3D-CT CFD model and the necessary properties of Large Eddy Simulation for computing urban transport and dispersion in complex geometry. Wind tunnel studies and field trials for validation of the CFD model and the CT-Analyst reduced order model are presented and discussed. The underlying idea behind nomografs is presented and the authors explain how conservative estimates of the agent contributions can also be determined quickly (i.e. in real time). Natural variability with regard to the validation field trials and the wind measurements is discussed. This 2013 publication is a "good read" and gives a detailed summary of the full range of wind tunnel and real-world experiments conducted in Hamburg to understand and validate both FAST3D-CT and CT-Analyst prior to their adoption for Hamburg's future operational use.

This paper concluded that it had become necessary to move to modeling techniques which can deal with the unsteady behavior of local scale dispersion in complex geometries in a more consistent way than previous methods. Technical progress meant the new generation of LES CFD models was ready for application to predictions for hazardous clouds resulting from accidental releases in urban or industrial environments. These LES models are computationally demanding but they can be applied before an emergency occurs. In combination with an intelligent tool which excerpts the relevant information from the simulated CFD results first responders receive immediate decision-making assistance.

CT-Analyst was held up as a prototype emergency management system adjusted to the geometry and validated for the city of Hamburg. In spring 2012 the new emergency management system was handed over to Hamburg's city authorities and has been tested under realistic operating conditions.

Flux-Corrected Transport Looks at Forty (invited review article), Jay Boris, *Computer & Fluids 84* 11312, 31 May 2013.

Abstract: The year, 2013, marked the 40th anniversary of the journal article "Flux-Corrected Transport I. SHASTA, A Fluid Transport Algorithm That Works" by Jay P. Boris and David L. Book [1]. Flux-Corrected Transport (FCT) removed a serious roadblock to advances in Computational Fluid Dynamics (CFD) by enabling the accurate treatment of strong, time-dependent shock problems in blast, reactive-flow, and combustion physics, and in aerodynamics and astrophysics. Steep gradients in conserved fluid variables could now be convected across a computational grid without the appearance of spurious oscillations and physically impossible negative values. The nonlinear "flux-correction" algorithm introduced in FCT imposes the physical monotonicity property of the convection equation without adding a great deal of numerical diffusion. This new "flux-correction" procedure, often called "flux-limiting," is the numerical principle underpinning most of the monotonicity-preserving, non-oscillatory, and total variation diminishing algorithms

that have appeared during these last four decades.

Comment: This is a invited review article about Flux-Corrected Transport, arguably my most widely used algorithm and software for Computational Fluid Dynamics. This paper became a vehicle to get NRL's broad and often referenced contributions again before the world community. For at least a few years the main FCT publication was NRL's most cited publication.

Airborne Puff and Plume Datasets for an Urban Landscape, J. P. Boris, M.-Y. Obenschain, K. Obenschain, Draft NRL Memorandum Report, March 2015.

Abstract: This report describes a database of "Puffs and Plumes" containing four high-resolution CFD datasets and associated files capturing the turbulent, time-dependent downwind evolution of ground-level tracer-gas clouds in a fictitious urban environment. Time histories of clouds from both continuous sources (plumes) and instantaneous sources (puffs) are presented. The database also contains files defining the urban geometry, a mask to overlay a 2D visualization of the geometry for display, and Fortran utilities to read and test the four compressed datasets. These datasets contain dense time sequences of ground-level tracer density fields from a uniformly spaced 1200x800 computational grid computed at 5-meter resolution. These density fields from both the "puff" and "plume" sources originate from six separate locations in the 6-km by 4-km urban domain. These datasets are structured to allow rapid analysis of turbulent fluctuations in the concentration of evolving puff and plume clouds and to study the naturally occurring variability expected between separate realizations of instantaneous releases in fluctuating wind fields. They can be used to assess the errors made in using time-steady models and other simplified representations of the urban fluid dynamics and they can be used to simulate proposed sensors and sensor systems in realistic airborne contaminant flows.

These four datasets were assembled from extensive CFD runs over a typical but fictitious urban landscape. FAST3D-CT, NRL's detailed Contaminant Transport (CT) model, was used to compute these databases. Field trials generally provide only a single realization of the flow and corresponding tracer cloud structure. However, in urban situations the difference between distinct realizations of the flow, determined for example by beginning each calculation at a different time, can be quite large. Even wind tunnel campaigns, which can provide many independent realizations, have difficulty going back and adding more data or refining a measurement after the limited-duration experimental campaign is complete. High-resolution, time-dependent, Large Eddy Simulation allows a class of scenarios to be revisited as often as desired to answer specific questions or to improve the statistics by collecting more data.

Comment: The Puff and Plume draft memorandum report is complete but fell by the way side because of a hang-up in getting the data released to be sent out if people requested it. I didn't follow up when security made this difficult and then became indisposed for essentially a year and a half.

Acute Exposure Guideline Levels (AEGLs) for Time Varying Toxic Plumes, J. Boris and G. Patnaik NRL/MR/6003-14-9493. September 2014.

Abstract: The U.S. EPA has established three Acute Exposure Guideline Levels (AEGLs) for predicting the onset of adverse health effects from inhaling specific duration exposures to specific concentrations of toxic chemicals for a general population. Most of this material is openly available on the internet (e.g. http://www.epa.gov/oppt/aegl, 2013). Further, a number of organizations, agencies and nations use these guidelines and may even mandate this approach to standardize estimating and reporting toxic health effects. The main drawback of the AEGLs is that only a few fixed-duration exposures to a few constant-density conditions are tabulated. The issue of how to treat real toxic plumes, whose agent density varies strongly and often quickly in space and time, is left undefined. Atmospheric transport and dispersion models provide estimations of a plume's movement and the associated agent density variations in 2D and 3D, but most crisis managers would like to see these results expressed in terms of the likely health effects – and get the information while there is still time to respond to and hopefully mitigate the threat.

We have developed a new algorithm and software to compute the onset of AEGL 1 (notable discomfort), AEGL 2 (irreversible or serious adverse impact), and AEGL 3 (life threatening or death) health-effects in response to general, time-varying concentration profiles that usually don't satisfy the specific constant-density-over-extended-period conditions expressed in the tabulated AEGLs. The AEGL 1, 2, and 3 onset conditions for any agent concentration history can be computed without reference to any particular pre-tabulated concentration or exposure duration. Plumes over entire urban areas can be integrated in fractions of a second, making this software implementation well suited to use with a dispersion model or CFD code.

Comment: This paper was also presented at the GMU Atmospheric Transport and Dispersion Modelling Conference. It allows detailed, accurate time-dependent integrations of toxic load accumulations using the underlying data of the EPA Acute Exposure Guideline Levels. Originally, we envisioned embedding the software in CT-Analyst to improve toxicity predictions. However, this approach did not take into account the wide range of likely exposure profiles that would be possible from different realizations of the same nominal agent-release scenario. These considerations eventually lead to the better (and faster) approach being developed in **Health Effect Hazard Areas for Airborne Contaminant Agents** below.

Proximity Analysis for Model Calibration and Validation, Jay Boris and Gopal Patnaik, U.S. Naval Research Laboratory (an unfinished NRL memo report), Jan 2015.

Abstract: This report describes a method to measure a multi-variable model's quality of fit to a given dataset in the same variables. We are adapting the name "Proximity Analysis" for these comparisons from techniques used in Geographical Information Systems, market research, and facility site selection, because the goals bare a resemblance and the name is singularly descriptive. The analysis methods are different, however, because the problems addressed are mathematically represented and often involve some aspect of physics or engineering.

Often one wishes to compare two or more distinct curves. Often the model or the data is represented as a multi-parameter curve. These curves may, for convenience, be represented as an ordered sequence of line segments. Sometimes the data consist of a cloud of data points as shown in the two-dimensional example of Fig.1 below. We are not concerned with how the test model is chosen initially or how the free parameters in the model are adjusted to minimize the difference between the model and the data set. Nor are we concerned with how to change the model representation itself when we perceive that the proximity of the model to the data is not as close as desired. We are only concerned here with how to measure the closeness, which we will call "proximity," between the data set and the model. Our interest in using a more general notion of proximity arose while developing a procedure to convert airborne puff and plume cloud configurations into simple polynomial shapes through a spatial coordinate transformation that captures the effect of complicated "urban" geometries on the shape of these time-dependent contaminant clouds. It is unlikely that all of this is new but there seems not to be a generally agreed, well-developed theory to use as a basis.

Comment: This report is all but complete and might well deserve journal publication. It certainly describes a potentially valuable new method to extract good analytic approximations from complex multidimensional data. It does, however, require a good, valuable real-world application to help make the case. It also suffers from the need for a method to extend the methodology to more than two or three dimensions. Perhaps the co-author could help finish this project.

The Shape of Tracer-Gas Clouds in Complex Geometry, Jay Boris and Gopal Patnaik, U.S. Naval Research Laboratory, January 2015.

Abstract: This report describes a compact method to represent spatially and temporally varying data describing tracer gas plumes in a complex-geometry environment such as a city. This representation is illustrated and validated using a detailed 3D Large-Eddy Simulation (LES) database constructed during a high-resolution numerical study. This database accurately captures naturally occurring density fluctuations with timescales down to 10 seconds in tracer gas clouds from instantaneous "puff" sources released at ground level. The methodology to evaluate and calibrate the compact representation involves performing "Proximity Analysis" to measure the differences between the multi-realization simulation data and an analytic model. This model arises as part of a procedure for transforming puff and plume data into an η–ζ (eta-zeta) coordinate system that captures the effect of complicated "urban" geometries on the shape of the airborne contaminant clouds.

Comment: This is an unfinished NRL memo report awaiting actual implementation of the resulting profiles in CT-Analyst.

Using Real-Time Chemical Plume Models in Virtual Training Systems, Adam Moses, Keith Obenschain, Dr. Jay Boris, Dr. Gopal Patnaik, 2015 IEEE International Symposium on Technologies for Homeland Security, Waltham, MA, April 14-16, 2015.

This paper describes the design, implementation, and use of integrated chemical plume-models in virtual training systems. The US Naval Research Laboratory has linked its CT- Analyst® software, a high-fidelity real-time plume modeling tool, with VBS2, a widely-used virtual gaming and training program, to produce new training capabilities that were previously unavailable. This work benefits two different but overlapping training scenarios: 1) tactical training for large-scale chemical gas attacks with a specific focus on crowd management, and 2) handler–focused training for users interested in working with IED-detecting dogs. The use of accurate, faster-than-real-time plume modeling enhances the virtual training systems to provide broader realistic support to the simulation and training communities.

Comment: As a result of the successes with CT-Analyst, ONR sought Code 6040 out for a program to develop a virtual-reality trainer for the handlers of IED-sniffing dogs in the middle east. This was a multi-million-dollar program over three years called Rover that we entered with Code 5580 for their expertise in programming virtual-reality actor motions. The work unit provided fluctuating plume models for CT-Analyst that allowed realistic tracking behaviors of the dog avatars as the scent fluctuated over the region of interest. The program was highly successful.

Health Effect Hazard Areas for Airborne Contaminant Agents, Jay Boris, Gopal Patnaik, and Keith Obenschain, Draft Report, May 2015.

Because inhalation toxicity usually depends nonlinearly on the contaminating agent density, time-dependent, naturally occurring density fluctuations in open-air release scenarios have a large effect on the overall symptom onset time. A wide range of toxic load integrals is found for different realizations of the same release. This natural variability makes integrating a model of a representative agent density time history time-history of relatively little value. Rather, the statistical distribution of possible toxic load integrals must be taken into account. What real-time users of a "predictive" model need to know is whether symptoms, at whatever health-effect level is being considered, can occur with unacceptably high probability and what is the earliest possible time this symptom onset can occur.

This paper reports a major simplification in computing these toxic agent health effects that accounts for the presence of large fluctuations. This new approach requires minimal agent time history data and also reduces uncertainty in the worst-case health-effect predictions. We show the distributions of possible toxic load integrals in terms of maximum density and earliest arrival time of the agent and how this information gives a simple, fast way to compute earliest symptom onset.

Comment: This is likely to be a very valuable contribution to the operational assessment of the threat of inhalation from airborne toxic agents under almost all threat conditions. It both explains an approach that unravels to difficulty arising from the wide natural variability of airborne threats while reformulating the problem in a way that gives first responders the information they really need in a crisis. The earliest time at which a given exposure symptom is likely to onset at each location is what a crisis manager or first responder really wants to know. This gives him, when computed as quickly CT-Analyst does, how much time he has, at each location in the threatened domain before the people in the local population begin to suffer from the exposure. This symptom onset time is subject to great physical variability from one ensemble realization to another so what the first responder needs is the plausible worst case to safe-side his actions. This new diagnostic meets the criteria exactly and is actually simpler to compute than using the EAGLE package previously described to integrate the concentration predictions in CT-Analyst. Funding to continue this important work has not yet been found.

Wind Tunnel Experiments or Advanced CFD ... What Do We Need for Understanding Flow and Dispersion in the Lower Atmospheric Boundary Layer? Bernd Leitl, Frank Harm, Eva Berbekar, Gopal Patnaik, Jay Boris, Michael Schatzmann, International Conference on Modeling Fluid Flows CMFF'15, Budapest, Hungary, 1-4 September 2015.

Abstract: Numerical modelling and physical modelling are often seen as competitors. Notably, this applies to the field of atmospheric physics and applied meteorology, where both types of models have to face severe restrictions with respect to the amount and complexity of physical processes to be captured in models. There is no doubt that substantial progress has been made, both in computational modelling and in the use of wind tunnels for simulating atmospheric flow and dispersion. Nevertheless, both approaches need to be combined in order to link model results with reality as it is measured. The paper illustrates some of the problems related to modelling and measuring flow and dispersion in the lower atmospheric boundary layer and intends to trigger at a conceptual level a discussion on how to combine specific strengths of both approaches to improve the understanding of flow and dispersion in the lower atmospheric boundary layer.

Comment: As part of the European COST project whose end result argued that RANS calculations of contaminant events were not reliable predictors of atmospheric agent releases, this paper went a long way toward illuminating what is thought to be the better, more scientific approach.

Hazmat Dispersion Modeling in Support of Urban Emergency Response for the Fire Brigade in Hamburg, Germany, E. Berbekar, F. Harms, B. Leitl, S. Fischer, J. Boris, A. Moses, K. Obenschain, G. Patnaik and K. Storm, Proceedings of 2016 IEEE International Symposium on Technologies for Homeland Security, Waltham MA, 10-12 May 2016, IEEE, 2016. Electronic ISBN: 978-1-5090-0770-7, Available at: http://ieeexplore.ieee.org /xpls/icp.jsp?arnumber=7568943.

Abstract: First responders need a more or less instant estimate of danger zones resulting from accidental airborne releases of hazardous materials in order to take immediate action, to coordinate rescue teams and to protect the population and critical infrastructure. To fulfill the need for efficient access to reliable results in a first responder's environment while maintaining sufficient dispersion modeling accuracy, pre-computed high-resolution CFD modeling can be combined with `physical data reduction' in an emergency assessment tool. This approach, specific to the geometry of the city of Hamburg, has been adopted by the Fire Brigade in Hamburg, Germany.

Comment: Our German colleagues attended a US conference presenting a version of the 2013 publication described above.

Local-Scale Hazmat Dispersion Modeling for First Responders Based on High-Resolution Computational Fluid Dynamics - an Overview of CT-Analyst Hamburg, Bernd Leitl, Frank Harms, Eva Berbekar, Jay Boris, Gopal Patnaik, Keith Obenschain, Susanne Fischer, Chemical Engineering Transactions, Vol 48, 2016, ISBN 978-88-95608-39-6, June 2016.

Accidental and deliberate releases of harmful substances pose a tremendous challenge to first responders because of the large number of possible casualties and the resulting potential environmental and economic damage in densely populated areas. Within minutes after a release, countermeasures must be taken to protect the population and environment adequately. This requires the exposed area, travel time of pollutants and possible exposure levels to be known in advance with sufficient accuracy in complex urban and industrial terrain where accidental releases are possible. This paper introduces an innovative and efficient concept for a more reliable local-scale hazmat dispersion modelling in the context of emergency response, developed at NRL. Using the current implementation of this approach for first response professionals in the city of Hamburg as an example, an overview of the emergency response tool

CT-Analyst Hamburg is presented. Unique features of the tool such as source location reconstruction based on available measured data or the simulation of pollutant retention time in built-up terrain are discussed. The extensive efforts undertaken to carefully and reliably validate the first responder's tool are described. Both, the underlying CFD-LES simulations as well as the CT-Analyst tool have been validated extensively using high-resolution test data sets generated in special boundary layer wind tunnel facilities and available field test data.

Comment: Our Hamburg collaborators have publication requirements much as we at NRL do. They prepare some publications that meet their requirements and interests and include us on many of them. Similarly, we include them on many of the papers we write. There is not 100% overlap since both organizations have different missions and goals. In particular, the University of Hamburg is more closely connected to their city than we are to D.C.

New Development: Synthetic Embedded Turbulence Integration Model, Jay Boris, Software Planning Document and Documentation, NRL Internal Documentation, July 2016.

Abstract: The goal is to build a Synthetic Embedded Turbulence Integration (SETI) for use in an LES-scale fluid dynamics model. This insert is a Lagrangian time-dependent model: 1) Driven by and adapted to the shears, rotations, and compressions of the resolved flow, 2) Hierarchical in terms of spatial and temporal scales, 3) Lagrangian in terms of fundamental representation (i.e. MLG-based), 4) Two-way coupled in both spatial scale and location, 5) Based on the nonlinear conservation laws of inviscid vortex dynamics coupled to a model of viscous-like dissipation at the shortest scales, and 6) Capable of efficiently generating a continuous, time-dependent high-resolution velocity field in the embedded domain. The model should be structured and optimized to allow at least a factor of 100 greater resolution than the effective CFD cell size. This will allow, for example, 10-cm UAVs to fly in turbulent flow fields computed on the 2- to 5-meter scale.

Comment: This report envisions, in a preliminary way, what the synthetic turbulence model might look like. This was the proposed end product of the work unit. In research, initial views and plans are often changed significantly. In this case, tackling the problem of non-equilibrium turbulence had to be done first, both for micro-UAVs in a urban environment and, as it turns out, for hypersonic flows. The Coherent Structure Dynamics model and the Cookie Cutter Mixing Model are the products that eventually surfaced in this effort. They are described in the last two reports of this document, **A Coherent Structure Dynamics Model for Non-Equilibrium Turbulence,** and **A Mixing Study Using Coherent Structure Dynamics.**

Neutralization of Airborne Contaminants, Jay P. Boris and Gopal Patnaik, AIAA Paper 2016–3196. Aviation 2016, Washington DC, AIAA, 13 June 2016.

This paper addresses the following question: Can an airborne cloud of a chemical or other unwanted agent in a populated region be neutralized effectively by injecting a suitable neutralizing “remediant” into the cloud in sufficient amounts and at appropriate locations? The outdoor transport and dispersion of potentially dangerous, contaminants is controlled principally by the wind, its turbulent gusts, and how this complex airflow interacts with the geometry of the buildings and terrain. The possible effectiveness of agent neutralization, or mitigation, is a complex matter of chemical reaction of the agent and the remediant, progressive dilution of the two reactants, and fluid dynamic mixing of the reactants over time. This paper presents a simple analytic solution, including dilution, chemical neutralization, and turbulent mixing, to estimate where and when to deliver the remediant and what amounts are necessary.

Comment: This theoretical paper was a spinoff of CT-Analyst applications for Hamburg. A closed form analytical equation relates the fraction of a toxic agent that could be neutralized (remediated) by injecting a neutralizing agent into the air following agent release to properties of the scenario and the assumed chemical reaction of the remediant and the agent. At best, the idea of after-release neutralization is an inefficient solution to the problem. The problem was suggested by chemical company salesman petitioning the DC emergency management people to position many tons of these chemical around Washington in the case of a toxic release. Further impetus was provided by discussion with AFOSR project officers but no funding materialized.

CT-Analyst Is Superior for Long-Range Transport and Dispersion, Jay Boris, (NRL internal software documentation, unpublished, August 2016.

Abstract: CT-Analyst is generally recognized as a superior transport and dispersion model for short-range and urban contamination scenarios. What is not generally known is the fact that it's advantages for urban, complex-geometry scenarios extend to and are even greater for transport and dispersion over much larger distances and longer times. There are several reasons for this.

1. The accuracy of the CT-Analyst model formulation does not degrade as distances and times are made larger because the effects of geometry on the evolving cloud shape are precomputed at the scale physically required. These effects are not "dumbed down" or averaged over to reduce the extensive "while you wait" computational delay of Lagrangian and Gaussian models.

2. Even over distances of tens and hundreds of kilometers the effect of local geometry on the impressed kilometer-scale wind fields is properly included in the hazard area and health effect computations near the ground where the spread of contaminant is most sensitive to the geometry and dangerous. CT-Analyst automatically transforms kilometer-scale meteorological wind fields to their actual behavior near the ground and in urban canopies so inaccurate flat-earth and random-walk approximations are avoided at all spatial scales, as opposed to most Lagrangian and Gaussian models.

3. The speed, but not the accuracy, of CT-Analyst is generally governed by how many pixels there are in the display, not by the resolution of the underlying Computational Fluid Dynamics (CFD) relative to how big the geographic domain is. Thus, scenarios can be computed and displayed in milliseconds, compared to minutes for other models, regardless of whether the region of interest is 2 km, 20 km, or 200 km in size.

4. CT-Analyst is based on time-dependent Large-Eddy Simulation and thus naturally occurring large-scale fluctuation effects, which continue to compound over long distances, are included directly in the formulation and precomputed accurately, as opposed to models based on the large-scale averaging of Reynolds Averaged Navier-Stokes (RANS) or even cruder approximations. The ever-present density fluctuations have a disproportionate influence on health effects because toxicity is usually a strongly nonlinear function of the local and instantaneous contaminant concentration.

5. CT-Analyst is state based, unlike other models, and thus no costly time integrations are performed. A one-hour (i.e. long distance) solution can be computed and displayed as quickly as 3 to 5-minute scenarios. This means that hundreds of scenarios with different source conditions, source types, and various different future wind fields can be inspected for their potential consequences by CT-Analyst during crisis management in the time it would take to compute a single solution by current standard methods.

Comment: This report never was published though it probably should have been. It was drafted in response to criticism of DHS contractors who wanted money for their Gaussian models. They were successful in deflecting DHS plans to support NRL CT-Analyst work further.

Contaminant Transport Analyst, S. Fischer, K. Storm, B. Leitl, G. Patnaik, J. Boris, F. Harms, E. Berbekar, Brandschutz Vol 70, p. 677, Sept. 2016, ISSN 0006-9094.

Abstract: Mit Contaminant Transport Analyst (CT-Analyst) verfügen die Siucherheitsbehörden in Hamburg seit Juni 2016 über eine innovative Software zur Prognose der Ausbereitung luftgetragener chemischer Substanzen ijm gesamten Stadgebeit sowie dem Hamburg Unland. Das auf einer Entwicklung des Forschungslabors der US-Marine beruhende Tool werde in zwei Sicherheitsforschungsprojekten unter maßgeblichter Beteiligung der Universität sowie der Fuerwehr Hamburg verbessert und für Einsatzzwecke in Deutschland aufgerüstet. Außer Feurwehren und Katastrophenschutzeinheiten gehören auch Betreiber von Industrieanlagen sowie Unwelt- and Gesundheitsbehörden oder Kommunen zu den moglichen von CT-Analyst.

Abstract: Since June 2016 using Contaminant Transport Analyst (CT-Analyst), the public health authorities in Hamburg have developed an innovative software package for forecasting the dispersion of airborne chemical substances in the entire city and state of Hamburg. The tool, which was based on developments of the US Naval Research Laboratory, will be improved in two safety research projects with the significant participation of the University and the Hamburg Fire Department and upgraded for use in Germany. Apart from fire departments and civil protection units, operators of industrial plants as well as environmental and health authorities or municipalities are among the possible recipients of CT-Analyst.

Comment: This short paper was published in the German fire brigade newspaper BrandSchutz and summarizes, for the target audience, work of the several previous papers.

LES validation of urban flow, part I: flow statistics and frequency distributions, Denise Hertwig, Gopal Patnaik, Bernd Leitl, Environmental Fluid Mechanics, 30 pages, Springer, DOI 10.1007/s10652-016-9507-7, December 2016.

Abstract: Essential prerequisites for a thorough model evaluation are the availability of problem-specific, quality-controlled reference data and the use of model-specific comparison methods. The work presented here is motivated by the striking lack of proportion between the increasing use of large-eddy simulation (LES) as a standard technique in micro-meteorology and wind engineering and the level of scrutiny that is commonly applied to assess the quality of results obtained. We propose and apply an in-depth, multi- level validation concept that is specifically targeted at the time-dependency of mechanically induced shear-layer turbulence. Near-surface isothermal turbulent flow in a densely built-up city serves as the test scenario for the approach.

High-resolution LES data are evaluated based on a comprehensive database of boundary-layer wind-tunnel measurements. From an exploratory data analysis of mean flow and turbulence statistics, a high level of agreement between simulation and experiment is apparent. Inspecting frequency distributions of the underlying instantaneous data proves to be necessary for a more rigorous assessment of the overall prediction quality. From velocity histograms, local accuracy limitations due to a comparatively coarse building representation as well as particular strengths of the model to capture complex urban flow features with sufficient accuracy are readily determined. However, the analysis shows that further crucial information about the physical validity of the LES needs to be obtained through the comparison of eddy statistics, which is focused on in part II. Compared with methods that rely on single figures of merit, the multi-level validation strategy presented here supports conclusions about the simulation quality and the model's fitness for its intended range of application through a deeper understanding of the unsteady structure of the flow.

LES validation of urban flow, part II: eddy statistics and flow structures, Denise Hertwig, Gopal Patnaik, Bernd Leitl, Environmental Fluid Mechanics, 28 pages, Springer, DOI 10.1007/s10652-016-9504-x, December 2016.

Abstract: Time-dependent three-dimensional numerical simulations such as large-eddy simulation (LES) play an important role in fundamental research and practical applications in meteorology and wind engineering. Whether these simulations provide a sufficiently accurate picture of the time-dependent structure of the flow, however, is often not determined in enough detail. We propose an application-specific validation procedure for LES that focuses on the time dependent nature of mechanically induced shear-layer turbulence to derive information about strengths and limitations of the model. The validation procedure is tested for LES of turbulent flow in a complex city, for which reference data from wind-tunnel experiments are available. An initial comparison of mean flow statistics and frequency distributions was presented in part I. Part II focuses on comparing eddy statistics and flow structures. Analyses of integral time scales and auto-spectral energy densities show that the tested LES reproduces the temporal characteristics of energy-dominant and flux-carrying eddies accurately. Quadrant analysis of the vertical turbulent momentum flux reveals strong similarities between instantaneous ejection-sweep patterns in the LES and the laboratory flow, also showing comparable occurrence statistics of rare but strong flux events. A further comparison of wavelet-coefficient frequency distributions and associated high-order statistics reveals a strong agreement of location-dependent intermittency patterns induced by resolved eddies in the energy-production range. The validation concept enables wide-ranging conclusions to be drawn about the skill of turbulence-resolving simulations than the traditional approach of comparing only mean flow and turbulence statistics. Based on the accuracy levels determined, it can be stated that the tested LES is sufficiently accurate for its purpose of generating realistic urban wind fields that can be used to drive simpler dispersion models.

Comment: These two papers present a necessary extension of the methodology needed for validating Large-Eddy Simulations of urban airflows in order to properly treat the intrinsic time dependence of turbulent urban flows. This new methodology makes use of wind tunnel data for model urban geometries that explicitly measures fluctuation statistics, including low-probability events. The two papers use the NRL LES model FAST3D-CT, providing the most complete and convincing validation of a such detailed CFD model to date. These papers are the substance of Dr. Hertwig's PhD Thesis from the University of Hamburg under Professor Bernd Leitl.

Blending Nomograf Regions for CT-Analyst®, Jay Boris, Adam Moses, Keith Obenschain, Gopal Patnaik, U.S. Naval Research Laboratory, Theodore Young, Jr., Berkeley Research Associates, Bernd Leitl, Frank Harms, Eva Berbekar, and Susanne Fischer, University of Hamburg and BIS Hamburg, June 2017.

Abstract: A Dispersion Nomograf™, or nomograf (NG) for short, is a multicomponent dataset that describes the effects that complex terrain and buildings have on the transport and dispersion of a contaminant cloud. A complete nomograf set has 18 pre-computed nomograf datasets, one for each of 18 nominal wind directions over an urban domain. Each NG dataset has two two-dimensional arrays which encode the downwind directions of the left and right edges of tracer gas clouds emanating from each point in the domain. This report describes an approach for constructing composite Dispersion Nomografs in rectangular domains that are described by blending several overlapping NGs prepared using CFD models with different resolutions and different geographic extents. These overlapping NGs may also be prepared by pre-computations using different fidelity models. We are considering domains having a few high-resolution NGs in which separate downtown (large building) areas may be embedded in broader areas having lower resolution that describe principally suburban and rural areas. We require an algorithm that transitions smoothly from one resolution CFD region to another while using the best (highest resolution, highest fidelity) CFD-based values where multiple CFD regions overlap. This procedure and the contributing algorithms are being designed to function for the new "nomograf-on-the-fly" representation implemented for plume evolution in CT-Analyst 5 and subsequent releases. Computational speed is therefore very important.

Comment: NRL patent attorneys suggested holding release of this work back for patent disclosure because of its importance to developing inexpensive, large-area nomografs. This patent slipped beyond the event horizon because of my illness. However, the likely impact is big. When larger coverage areas are required, only the new area need be computed with FAST3D-CT. The two CFD computations can be blended into a composite larger area seamlessly. When a few buildings are modified or added to a landscape they can be added to the overall nomografs by a small local 3D computation set rather than having to recompute the entire area. Computations at different resolution can be blended so a large low-resolution area can provide a useable background for injection of higher-resolution downtown areas, local facilities, and industrial plants. These high-resolution areas can be added at any time so the quality of the representation can be upgraded, for example, when better geometry data becomes available. This capability opens the way to country-scale and continental-scale application of CT-Analyst technology.

On the simulation of wind-driven hazardous material dispersion in complex built-up terrain - Potential and drawbacks of dispersion modeling, B. Leitl, K. Storm, S. Fischer, F. Harms, J. Boris and G. Patnaik, *Journal for Research, Technology and Management in Fire Protection*, Issue 3/2017, Vol 66, No. 3, August 2017, page 144–158 (original in German).

Abstract: The release and the wind-driven transport of hazardous substances as a result of industrial accidents, fires or - much less often - criminal attacks are particular challenges for rescue and rescue teams. Typical for the frequently localized accident scenarios are comparatively short release and propagation times. In addition to measuring and tracing technology, the reliable and rapid prediction of the spread of hazardous substances in space and time is of central importance in the technical support of operational management. For this reason, quite a number of software tools have existed for quite some time; The corresponding research and development has been significantly boosted technically by the developments in the IT area and in terms of content by the terrorist threat since 2001.

The article first describes three basic types of dispersion models, their advantages and their application limits, which are mainly used in air quality and incident management. As part of an international research project, various software tools based on the basic types and used in incident management were compared. The article gives an overview of the basic results of this comparison. Subsequently, an innovative fourth approach and a conceptually new application tool for the propagation simulation based on it, which has been continuously researched by scientists and users in Hamburg and Washington D.C. was further developed. The simulation tool "CT-Analyst Hamburg" permits the reliable and, above all, very fast prediction of hazardous substance spreading processes even within densely populated urban and industrial structures.

Comment: This journal article places in context the joint efforts of the collaboration between the University of Hamburg team and the NRL CT-Analyst team. It was written for the German Journal of Research and Technology in Fire Protection to reach their professional audience. Professor Leitl lead the European COST Action Group studying urban transport and dispersion. This paper was, in part, his summary of finding that Large Eddy Simulation (LES) models are superior to Reynolds-Averaged Navier-Stokes (RANS) models for modeling contaminant transport in cities.

Modeling Atmospheric Contaminant Transport for Real-Time Response in Cities, J. Boris, S. Fischer, K. Storm, G. Patnaik, D. Hertwig, B. Leitl, F. Harms, A. Moses and K. Obenschain, *journal article in preparation*, September 2018.

Abstract: The release and wind-driven transport of hazardous substances, resulting from industrial accidents, fires, or - much rarer - criminal attacks, are special challenges for first responders, crisis managers, and rescue workers. This paper discusses the evolution of these threats from the perspective of how the real-time response to such airborne Contaminant Transport (CT) emergencies in cities can be aided by transport and dispersion modeling that satisfies real-world speed and accuracy requirements. Incident response personnel usually need their modeling questions answered in about the time it takes to ask the question – a few seconds. In this paper, we also describe an urban prediction model CT-Analyst® that was designed specifically to contribute to a time-limited response during an information-poor emergency. In urban applications, CT-Analyst is faster and more accurate than other modeling approaches while being flexible and easy to use.

Comment: The publication of this journal article is being delayed by two factors: 1) getting input from all the authors in a timely way and 2) what journal to send it to? It wants to be something the fire and hazmat professionals will actually read and therefore is outside our experience range as authors.

A Coherent Structure Dynamics Model for Non-Equilibrium Turbulence, Jay Boris, U.S. Naval

Research Laboratory, NRL/MR/6003–18–9815, September 2018, also to be submitted as a journal article.

Abstract: This paper introduces a computational model that computes the time-dependent evolution of a non-equilibrium turbulence spectrum from the system size down to the viscous dissipation scale. Turbulence models for use with Computational Fluid Dynamics (CFD) have at best treated the inertial-range below the CFD resolution as if obeying a renormalizable or scale-similar equilibrium described by the Kolmogorov spectrum with a spectral energy density that scales as $k^{-5/3}$. The "Coherent Structure Dynamics" (CSD) model introduced here addresses situations where the time-scale for changes in the macroscopic fluid dynamics is short and thus the resulting turbulence is far from an equilibrium cascade because the turbulent small scales that drive the dissipation will not have had time to equilibrate. Such circumstances can be caused, for example, by strong shocks passing through passive density gradients or fuel injection into supersonic flows. Mixing on the molecular scale and thus chemical reactions will be delayed until the short scales in the velocity spectrum are energized.

The CSD model is not derived from the Navier-Stokes equations. It is constructed to satisfy the important physical conditions of the problem including scale consistency of the inviscid, nonlinear, fluid-dynamic interactions between the coherent structures that actually comprise turbulence. In addition to treating the kinetic energy density as a function of scale size down to the Kolmogorov dissipation scale, a number density of coherent structures at each scale is introduced to account for the fact that the relative spacing of the structures comprising turbulence, particularly away from equilibrium, may not be the same at all scales. This dynamic system relaxes to the Kolmogorov spectrum with a definite pre-dissipative bump (the bottleneck). Two scale-independent parameters in the model are calibrated using the Taylor-Green vortex problem. Examples are presented and tests of the model are discussed.

Comment: This paper describes a new representation and numerical model, called Coherent Structure Dynamics (CSD) for solving the time-dependent evolution of complex, non-equilibrium turbulence spectra from macroscopic scales to past the dissipation scale. Since Detailed Numerical Simulation is not required, CSD is orders of magnitude faster than previous methods and, at the same time, allows treatment of a much wider range of spatial scales. This paper is published first as an NRL Memorandum Report to assure a time stamp on the ideas and results. This paper will soon be "journalized" but the appropriate journal is being debated: Journal of Fluid Dynamics Research, Computers and Fluids, Physics of Fluids, Journal of Computational Physics? Each of these has different, and rather horrific, publication requirements.

A Mixing Study Using Coherent Structure Dynamics, Jay Boris, Draft of a U.S. Naval Research Laboratory Memorandum Report.

Abstract: This paper uses a reduced-order "Coherent Structure Dynamics" model, introduced in an earlier paper, to compute the time-dependent interspecies mixing due to a non-equilibrium turbulent spectrum. The Coherent Structure Dynamics (CSD) model addresses situations where the time-scale for changes in the driving fluid dynamics is short and thus the resulting turbulence may be far from equilibrium because the turbulent small scales will not have had time enough to populate. True molecular mixing and thus chemical reactions will be delayed until the short scales in the velocity spectrum have been energized. Realizations of the turbulence from the CSD model

are applied to a triply-periodic cube of a tracer density to study the mixing of two chemical species. This calculation measures the time delay in molecular-scale mixing caused by the delayed population of the short wavelength turbulent scales that bring the two species close enough to mix molecularly. A Direct Numerical Simulation (DNS) of such mixing in a Reynolds-number 1 million flow might require 10^6 x 10^6 x 10^6 computational cells if uniformly resolved. Subgrid turbulence models for use with Computational Fluid Dynamics (CFD) have generally treated the inertial-range below the CFD-resolved scale as if obeying a renormalizable or scale-similar equilibrium described by the Kolmogorov spectrum with a spectral energy density that scales as $k^{-5/3}$ in the inertial range. This assumption is only relevant when the turbulent spectrum is in or near an equilibrium energy cascade.

The CSD model is a new approach, based on the nonlinear interaction of the coherent, fluid-dynamic structures that comprise turbulence. The kinetic energy density as a function of scale size is resolved on a logarithmic grid to describe the entire turbulent spectrum. In addition, a number density of coherent structures at each scale is introduced to account for the fact that the relative spacing of the coherent structures, particularly away from equilibrium, may not be the same at all scales. Two cases are used to study and compare the small-scale mixing: 1) an equilibrium turbulence spectrum driven by constant stirring at the system scale and 2) a highly-transient non-equilibrium case where the stirring at the system scale is the only non-zero component of the spectrum initially. The details of the CSD formulation and the numerical algorithms are discussed in an earlier paper. Here a diffusion-free "Cookie-Cutter Density" model is used to instantiate the CSD time-dependent spectrum as a surrogate flow field capable of driving turbulent mixing.

Comment: As with the previous report, there is some concern with stamping NRL's precedence here. Also, this work has to be finished as this is the most recent of the Coherent Structure Dynamics activities. A number of slight improvements to the Cookie Cutter Model suggest themselves and are gradually being followed up.

III Summary: The several papers, reports and drafts describing new innovations, research results and capabilities from the work unit that seem most important, as leveraged by and leveraging the efforts of our German colleagues, are now listed.

The How and Why of Nomografs™ for CT-Analyst® (Jay Boris) presents the structure and reasoning behind nomografs and how they enable both great speed and accuracy in CT-Analyst.

Using Real-Time Chemical Plume Models in Virtual Training Systems (Adam Moses, et al.) describes the design, implementation, and use of integrated chemical plume-models in virtual training systems. CT- Analyst®, a high-fidelity real-time plume prediction tool, with VBS2, a widely-used virtual gaming and training program, to produce new training capabilities that were previously unavailable. This work benefits two different but overlapping training scenarios: 1) tactical training for large-scale chemical gas attacks with a specific focus on crowd management, and 2) handler–focused training for users interested in working with IED-detecting dogs. The use of accurate, faster-than-real-time plume modeling enhances the virtual training systems to provide broader realistic support to the simulation and training communities.

As a result of the successes with CT-Analyst, ONR sought Code 6040 out for a program to develop a virtual-reality trainer for the handlers of IED-sniffing dogs in the middle east. This was a multi-million-dollar program over three years called Rover that we entered with Code 5580 for their expertise in programming virtual-reality actor motions. The work unit provided fluctuating plume models for CT-Analyst that allowed realistic tracking behaviors of the dog avatars as the scent fluctuated over the region of interest. The program was highly successful.

Acute Exposure Guideline Levels (AEGLs) for Time Varying Toxic Plumes (Jay Boris & Gopal Patnaik), describes the EAGLE software package that properly interpolates the EPA AEGLs (Acute Exposure Guideline Levels) for all timescales and toxic agent densities, allowing integration of the toxicity and symptom onset time for any smooth or fluctuating agent time history. We do not see incorporating this software in NRL's operational airborne contaminant transport package, CT-Analyst, because extensive use of EAGLE for hundreds of thousands of real-world scenarios helped elucidate a much better algorithm. This algorithm, introduced in the report, **Health Effect Hazard Areas for Airborne Contaminant Agents**, is faster still and included the effects of an ensemble of realizations giving first responders exactly what they need, the earliest symptom onset time at each location.

Characterization of Transient Dispersion Processes in An Urban Environment (Frank Harms, et al.) and **Wind Tunnel Experiments or Advanced CFD ... What Do We Need for Understanding Flow and Dispersion in The Lower Atmospheric Boundary Layer?** (Bernd Leitl, et al.) These papers illustrate the evolution of Hamburg's cutting edge experimental wind-tunnel technology for analyzing urban air flows. During the DTRA sponsored project related to the Oklahoma City field trials, it became apparent that multi-realization analyses were crucial to understanding the range of possible results that could occur in a given atmospheric flow.

LES validation of urban flow, part I: flow statistics and frequency distributions, (Denise Hertwig, et. al.) and **LES validation of urban flow, part II: eddy statistics and flow structures**, (Denise Hertwig, et. al.) extended the validation methodology for application to Large-Eddy Simulation models

Blending Nomograf Regions for CT-Analyst® (Jay Boris, et al.) presents a new technique, realized in operational software, to take separate CFD calculations of different areas and at different resolutions and blends them efficiently into a larger more inclusive CFD coverage of an urban region. This innovation allows the piece-wise assembly of huge high-resolution regions of CT-Analyst coverage. Extension to country-wide and continental-scale nomograf databases at high resolution is made possible.

A Coherent Structure Dynamics Model for Non-Equilibrium Turbulence (Jay Boris). This paper describes a new turbulence representation and numerical model, called Coherent Structure Dynamics (CSD), for solving the time-dependent evolution of complex, non-equilibrium turbulence spectra from macroscopic scales to past the dissipation scale. Since Detailed Numerical Simulation is not required, CSD is orders of magnitude faster than previous methods and, at the same time, allows treatment of a much wider range of spatial scales.

A Mixing Study Using Coherent Structure Dynamics (Jay Boris) is the second CSD paper and is still in preparation. It uses the non-equilibrium spectrum from CSD to drive a single realization of "fluid flow" in a cubical domain to compute the mixing of two initially separate species. This idealized surrogate fluid problem is designed to get at the fundamentals of high Reynolds number mixing for application to turbulent combustion.

Acknowledgements: The principal investigator of this work unit wishes to thank his NRL colleagues Gopal Patnaik, Keith Obenschain, and Adam Moses for their scientific contributions to the research conducted on "Highly Complex Fluid Dynamics" in the NRL 6.1 Base Program. He also wishes to thank Drs. Kazhikthra Kailasanath, David Mott and Fernando Grinstein, and Professors Alexei Poludnenko and Elaine Oran for their helpful discussions and critical comments. This work was supported in principal part by ONR through the NRL 6.1 Base Program.