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Overview of LDRD project 05-ERD-050: "Developing a Reactive Chemistry Capability for the NARAC Operational Model (LODI)"

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Disclaimer

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Purpose of project

The primary purpose of this project was to provide LLNL/NARAC the ability to simulate arbitrary networks of chemical reactions within their emergency response atmospheric dispersion model (LODI), so that it can handle the reactions relevant to species such as nerve agents, chlorine, and ozone, plus the *in situ* creation of aerosols from species such as oleum and UF_6. This is a unique emergency-response capability that greatly enhances the LLNL/NARAC ability to respond to terrorist attacks and industrial accidents that involve reactive chemistry. This capability will also facilitate detection and monitoring plans for factories and laboratories, including clandestine facilities. The resulting model also has a dual potential for local and regional air-quality studies.

Summary of Results

We developed and implemented the capability to simulate arbitrary networks of chemical reactions within the LLNL/NARAC emergency response atmospheric dispersion model (LODI), so that it can handle the reactions relevant to nerve agents, chlorine, ozone, and the in situ creation of aerosols from species such as oleum (SO_3) and UF_6. We also went further than our original plans and developed the capability to calculate the heat generated from chemical reactions and aerosol formation, which can be sufficient to cause a cold and dense plume hugging the ground to rise into the atmosphere, then descend to the ground again as droplets.

In particular, we developed and implemented into the LODI model: (1) the semi-Lagrangian advection scheme we developed, (2) our aerosol dynamics capability, (3) a Gear general chemistry ODE solver, (4) our chemical mechanisms for chlorine, oleum, ozone, and nerve-agents, and (5) the ability to track the heat generated from chemical reactions and aerosol formation. As an incidental benefit, we improved the multi-processor scaling and memory usage of LODI in order to expedite the simulations for emergency response. We spent a lot of time interacting with the NARAC development team to educate them on the principles and capabilities we developed. We also worked them on the migration of our improvements into the main LODI code base, and that effort is continuing.

The main report is provided in "*Final Report for LDRD project 05-ERD-050: Developing a Reactive Chemistry Capability for the NARAC Operational Model (LODI)*" (LLNL-TR-401274). A detailed description of the aerosol capability we developed and

implemented is provided separately in "*An Aerosol Condensation Model for Sulfur Trioxide*" (LLNL-TR-401137).

Auspices

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