Major science issues in atmospheric transport and dispersion modeling of accidental releases of ammonia to the atmosphere

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Ammonia is usually stored as a liquid by refrigerating it to its boiling point (-34 C), or as a pressurized liquefied gas at ambient temperatures. Other papers at this workshop will address stakeholder concerns, release scenarios, emissions calculations, and exposure and health assessments. The subject of this paper is atmospheric transport and dispersion (ATD) models, which use inputs of the specified emissions conditions (at the point where the ammonia reaches ambient pressure) and produce outputs of concentration distributions over time and space, which are provided to the exposure and health models. The ATD model can include density effects (either buoyant plume rise or dense gas slumping), chemical reactions, ambient water and ammonia droplet evaporation and condensation, and deposition to the surface.

Much current research is underway on ammonia's contributions to air pollution, and several new models are available (e.g., regarding ammonia's reactions with sulfates and effects on visibility). However, the ammonia concentrations resulting from routine emissions sources (e.g., cattle feed lots) are generally a few ppb, which are much less than concentrations associated with ammonia accidents (several ppm or more). Consequently. the information from the ammonia air pollution studies is not always relevant to accidental releases.

This paper provides an overview of the science issues addressed by ATD models applied to accidental releases of ammonia, the differences between operational (emergency response) and research applications, the types (with examples) of available ATD models, pros and cons of specific ATD models (including DEGADIS, SLAB, HPAC/SCIPUFF, CAMEO/ALOHA, QUIC, MSS, PHAST, FLACS, and AEOLUS), and examples of evaluations of ATD models with available ammonia field experiment data (e.g., FLADIS and Desert Tortoise pressurized releases, and Frie et al. small-scale evaporating pool).