VERIFICATION

UDM THERMODYNAMICS

DATE: December 2023

This verification manual describes the verification, validation and sensitivity analysis for the thermodynamics in the Unified Dispersion Model (UDM).

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1 INTRODUCTION

This verification manual describes the verification, validation and sensitivity analysis for the thermodynamic modules in version 6.0 of the Unified Dispersion Model (UDM) implemented into the DNV software package PHAST 6.0. the individual modules in version 6.0 of the Unified Dispersion Model (UDM). Each of the thermodynamic modules has been investigated in detail in conjunction with a literature review and a sensitivity analysis. The modules have been corrected where necessary, validated where possible, and been compared with external models like the Shell package HGSYSTEM.

The subsequent chapters in this report investigate the following.

1. Two-phase non-reactive equilibrium thermodynamics model (liquid temperature = vapour temperature) for mixing of pollutant with moist air. This includes the effects of the presence of separate aerosols for pollutant and water. Also heat and water vapour transfer from the substrate is discussed.

2. Two-phase equilibrium thermodynamics model (liquid temperature = vapour temperature) for mixing of hydrogen fluoride (HF) with moist air. This includes the effects of polymerisation and the formation of an aqueous fog.

3. Assessment for the droplet non-equilibrium thermodynamics (liquid component temperature below vapour temperature). This includes calculation of droplet trajectories, droplet mass and droplet temperature.

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