1. GENERAL INTRODUCTION

1.1. Introduction

This Technical Reference Manual gives technical background information for the HGSYSTEM version 3.0 models. To keep this Manual as concise as possible, in general only that information is supplied which is not available in the open scientific literature.

Of course, for every model detailed descriptions of all input parameters is given in the HGSYSTEM User's Manual. Information in the User's Manual should enable the user to run any HGSYSTEM model.
The information in this Technical Reference Manual is intended as supplementary information for those users who want to know more about the 'technical' contents of an HGSYSTEM model.

In this paragraph, an overview of the main new features available in HGSYSTEM version 3.0 is given, as compared to the first public domain release of HGSYSTEM, version 1.0 which is also called the NOV90 version.

1.2. Main new features in HGSYSTEM version 3.0

Compared to the first public version of HGSYSTEM (version 1.0 or NOV90), many changes have been made to the separate models. Apart from several minor changes (additional input parameters, removed bugs etc.), the following new *major features* are now available in version 3.0 of HGSYSTEM.

- A new thermodynamical model describing *multi-compound, two-phase fluids* has been implemented. This model is also called the HGSYSTEM aerosol model. It is described in full detail in Chapter 2.A. It is available in all main and non-HF specific HGSYSTEM models.

- To generate the physical compound properties need by the new two-phase model, a *database program* called DATAPROP has been added to HGSYSTEM. DATAPROP generates link files containing all relevant data, for all HGSYSTEM models using the two-phase description.

- The new PLUME version using the new two-phase thermodynamical model is renamed to *AEROPLUME*. AEROPLUME describes near-field jet dispersion for multi-compound, two-phase releases from pressurised vessels. AEROPLUME has a built-in discharge model

to give estimates for release rates, that is, it calculates a source term for the dispersion calculation.
The AEROPLUME implementation in HGSYSTEM is described in detail in Chapter 5.A.

- The *hydrogen fluoride (HF) chemistry and thermodynamical model* has been extended to describe mixtures of HF, water and an inert ideal gas. This model is now available in the HGSYSTEM modules HFPLUME, HEGADAS and the new HEGABOX model. The new HF model is described in full detail in Chapter 2.B.

- A new model describing the initial gravity slumping behaviour for *instantaneous releases* is now available in HGSYSTEM. This model is called HEGABOX. More details are given in Chapter 8.

- A new model calculating the *transient* (time-dependent) *release rate* of a multi-compound, two-phase fluid from a pressurised vessel is now available in HGSYSTEM. This model is called SPILL and can be seen as the counterpart of the HF-specific model HFSPILL. The new SPILL model is discussed in full detail in Chapter 3.

- The EVAP model describing *evaporating liquid pools*, as used in HGSYSTEM 1.0, has been replaced be a completely new model called LPOOL. LPOOL is based on the LSM90 model as made available by Exxon Research & Engineering Company. LPOOL can be used for boiling and non-boiling pools of multi-compound mixtures on land or on water. More information on the LPOOL model is given in Chapter 4.

- The HEGADAS algorithm has been revised to prevent unrealistic concentration profiles. A detailed description of these changes is given in Chapter 7.B.

- Several new options have been added to the transient (time-dependent) version of the heavy gas model, HEGADAS-T. These new features are:
  - An algorithm to automatically generate an 'optimal' set of output times. See User's Manual, Chapter on HEGADAS, input block AUTOTIM.
  - A similar algorithm to automatically generate an 'optimal' step size in the downwind direction. See User's Manual, Chapter on HEGADAS, input block CLOUD, parameters XSFACT and XSEPS.
  - The possibility to specify a change in surface roughness at given downwind distances. See User's Manual, Chapter on HEGADAS, input block TRANSIT, parameter ZRS.
    Technical documentation on these new HEGADAS-T features are given in Chapter 7.C.

- The post-processors for HEGADAS results have been updated and can now be used in 'batch' mode like all other main HGSYSTEM modules. Capabilities for dosage calculations were added. Time-averaging is now done in a better way. These new models are called POSTHS and POSTHT. See the relevant chapter in the HGSYSTEM User's Manual.

- A utility program to generate concentration contours for airborne plumes as calculated by AEROPLUME and PGPLUME, is now available. The utility is called PROFILE. See the relevant chapter in the HGSYSTEM User's Manual.

- The model HFJET, which was a strongly simplified version of the HFPLUME model, is no longer part of HGSYSTEM, as its use is very limited.

- Following work done on a specific HGSYSTEM version by The Earth Technology Corporation, U.S.A., several new options are now available to all users of HGSYSTEM version 3.0. This work was sponsored by Martin Marietta Energy Systems and the added options are therefore available in an MMESOPT input block. The technical descriptions of options are given in Chapter 9. The corresponding input parameters are discussed in the HGSYSTEM 3.0 User's Manual for the relevant models (AEROPLUME, HEGADAS, HEGABOX and HFPLUME). General guidance is given in Chapter 18 of the HGSYSTEM 3.0 User's Manual.