8. THE HEGABOX MODEL

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Error! Bookmark not defined.**.1. Introduction**

The first public domain release of HGSYSTEM (version 1.0 or NOV90), contained a range of models to simulate the different aspects of an hazardous release. However, a model to describe the initial phase in the spreading of an initially stagnant, dense cloud was not yet available within this first HGSYSTEM version. The second public domain release, HGSYSTEM version 3.0, does now contain such a model, called HEGABOX, and in this chapter some background information for this new HGSYSTEM model will be given.

The HEGABOX box model was available as a stand alone model since it was developed [1,2], but has been incorporated into HGSYSTEM version 3.0, completely analogous to and compatible with the other HGSYSTEM models. HEGABOX is linked with the database program DATAPROP and the far-field time-dependent heavy gas dispersion model HEGADAS-T, both available within HGSYSTEM.

The two standard HGSYSTEM thermodynamical descriptions are available in HEGABOX: a multi-compound, two-phase, non-reactive model and a model containing the full reactive hydrogen fluoride (HF) chemistry and thermodynamics.

In this chapter a global description of the HEGABOX model is given as well as a discussion on its implementation into HGSYSTEM.

Error! Bookmark not defined.**.2. Model description**

The HEGABOX model was developed by Puttock to describe the transient dispersion behaviour of instantaneous 'box' releases of heavy gases. Details of model assumptions are given in [1,2], here only a global description is given.

HEGABOX describes the gravity-dominated phase of the dispersion of a suddenly released amount of heavy gas which initially has no momentum of its own. In this phase *slumping* caused by gravity and the (strongly time-dependent) mixing associated with this phenomenon, are dominant. The scenarios which can be simulated using HEGABOX are dense gas releases at low wind speeds or the sudden release of a large quantity of a dense gas

For an instantaneous release or a release at low ambient wind speeds, not only the *gravity-driven lateral spreading* of the cloud is important, but also the *gravity spreading* and *slumping* along the wind direction. The model takes both these effects into account.

HEGABOX assumes the cloud to have a cylindrical shape and the pollutant concentration is assumed to be uniform within the cylinder.

After the release, the cloud radius R will start growing due to the gravity-driven slumping of the dense cloud. The cloud height H will initially decrease (R increases), but eventually H will increase due to *entrainment* of ambient air. Entrainment is caused by the slumping of the cloud (principally at the cloud edge), but there is also entrainment through the top of the cylindrical cloud.

The cloud (bulk) velocity, which is initially zero, will start to increase as momentum from the ambient air is imparted to the cloud. For longer times the cloud will move with the ambient wind speed.

After this initial phase, the influence of ambient turbulence on the pollutant dispersion becomes more and more important with increasing time. Spreading in the wind direction by gravity slumping becomes much less important than the spreading caused by the cloud's own speed, which for longer times will be equal to the ambient wind speed. HEGABOX does not take these effects into account and therefore we should make a transition from HEGABOX to a far-field model to adequately simulate the cloud behaviour for longer times. In HGSYSTEM this model is the transient version of far-field heavy gas model HEGADAS-T.

Error! Bookmark not defined.**.3. Implementation in HGSYSTEM**

Error! Bookmark not defined.**.3.1. Thermodynamics**

In line with the other major HGSYSTEM modules the pollutant in HEGABOX can be either a non-reactive two-phase mixture consisting of several compounds or a reacting aerosol of HF, water and an inert gas. Pure ideal gas calculations are a special case of the non-reactive aerosol thermodynamical model. It is thought that this flexibility will make it possible to apply HEGABOX simulations to a wide range of pollutant releases.

To facilitate the use of HEGABOX with more complicated pollutant compositions (with or without HF), the HGSYSTEM database program DATAPROP can be used prior to a HEGABOX calculation. DATAPROP produces a link file with HEGABOX input parameters (GASDATA block) in a similar way as it does for other HGSYSTEM modules.

Error! Bookmark not defined.**.3.2. Initial conditions**

The initial cloud size for any HEGABOX simulation is determined from fluid properties (using the relevant thermodynamical model), the user-specified spill size and a user-specified initial radius. In calculating the initial cloud size, HEGABOX assumes that all liquid (if any) is dispersed as a fine mist (aerosol) throughout the cloud.

Problems with significant liquid pools on the ground cannot be dealt with, liquid dropout from the cloud to the ground is not being modelled. If the initial cloud composition as found by HEGABOX results in a cloud with a very high liquid fraction then increasing the user-specified initial entrainment (see discussion on input parameters) might be helpful.

In the report file the user can check whether the liquid mole fraction in the cloud exceeds reasonable values. It is the user's responsibility that aerosol liquid fractions are not too high as to violate model assumptions (no dropout, liquid finely dispersed).

The initial cloud temperature has to be specified by the user and it will in general be different from ambient temperature. It could be the result of a flash calculation. The cloud pressure is taken to be equal to the ambient pressure and in HEGABOX (just as in HEGADAS) this is always taken to be 1.0 atm (760 mm Hg).

Heat transfer and convective entrainment are included in a similar way as in HEGADAS.

Error! Bookmark not defined.**.3.3. Transition to far-field model**
After calculation of the early stages of the cloud dispersion, HEGABOX has to make a smooth transition to the far-field heavy gas dispersion model available within the HGSYSTEM environment to allow a more accurate and detailed description of the dispersion process for longer times. As the HEGABOX release scenario is strongly time dependent, a transition is made to the transient variant of the HEGADAS model, HEGADAS-T, rather than to the steady state version.

A transition can be made if the influence of gravity-spreading no longer dominates as strongly as in the initial phase compared with the spreading due to the cloud's own velocity. The relevant dimensionless group, comparing the gravity forces with the inertia forces, is the Richardson number (Ri). In general it is defined as

$$Ri = \frac{g \cdot \Delta\rho \cdot L}{\rho \cdot (\Delta u)^2} \qquad (1)$$

where g is the acceleration of gravity (m/s^2), ρ a density (kg/m^3), $\Delta\rho$ a density difference (kg/m^3), L a length scale (m) and Δu a velocity difference (m/s).

The transition from HEGABOX to HEGADAS-T occurs when the Richardson number based on an internal cloud velocity, drops to a specified value (default value is 10, can be changed by the user). This 'critical' Richardson number Ri* is defined as

$$Ri* = \frac{g' \cdot H}{(u*)^2} \tag{2}$$

where g' is the reduced gravity defined by

$$g' = g \cdot \frac{\rho - \rho_a}{\rho_a} \tag{3}$$

where ρ is the cloud density (kg/m^3), ρ_a the ambient density (kg/m^3) and g the acceleration of gravity (m/s^2).
Further in (2), H is the cloud height and u* is an internal velocity scale defined as

$$u* = \frac{\kappa \cdot U_b}{\log(H / z_r) - 1} \tag{4}$$

where κ is the von Kármán constant (value 0.41), z_r the surface roughness length and U_b the cloud bulk velocity. For more details see [1,2].

Thus the HEGABOX simulation ends when the value of Ri* falls below the pre-set transition value which has a default value of 10. This is the normal way of ending a HEGABOX run.

At the end of each run, HEGABOX prepares a link file which contains input parameters used by HEGADAS-T, completely in line with the normal HGSYSTEM approach. Apart from this link file, HEGABOX also prepares a file containing observer data, which HEGADAS-T needs to continue the dispersion simulation. Details on how the observer data are being calculated and on assumptions made when linking to HEGADAS-T, can be found in [1,2].

A complete simulation, involving consecutive runs of DATAPROP, HEGABOX and HEGADAS-T, can be made using either the interactive environment HGINTER or using HGSYSTEM in the batch mode (for more experienced users) and this can be done for pollutants with or without HF.

Error! Bookmark not defined.**.4. Model validation**

When preparing the HGSYSTEM version of HEGABOX, the results of several HEGABOX runs using the original HEGABOX thermodynamic routine were compared with the older mainframe run results and they were found to be close, as they should be. Results are not identical because of updates in HEGADAS-T and the thermodynamical routines. Differences are generally less than 2 %.

Puttock in [1] made a detailed comparison between HEGABOX/HEGADAS-T and the experimental results obtained at Thorney Island. He found a quite good agreement between predictions and experiments.

As the HGSYSTEM implementation for these cases (ideal gas thermodynamics) is principally the same as the model used by Puttock, it is concluded that the current HGSYSTEM models HEGABOX and HEGADAS-T are in very good agreement with the Thorney Island data.

To demonstrate this we take as an example trial number 16, which is a typical Thorney Island run. We only consider HEGABOX results here. Observed data and results of previous HEGABOX runs are taken from [1]. The predicted average cloud speed 8-16 seconds after the release is 1.84 m/s (old mainframe version) or 1.97 m/s for the HGSYSTEM model. The observed value is 1.80 m/s.

We can also look at the distances required for a certain decay of peak pollutant concentration. To reach a concentration of 5 %, the observed distance is 120 m, the old model predicts 157 m and the current HGSYSTEM model predicts 156 m. For a decay to 2.5 %, the experimental distance is 205 m, the old model predicts 243 m and the HGSYSTEM version 242 m. To reach 1 % the observed distance is 370 m, the old model gives a distance of 380 m and the new version predicts a value of 386 m.

For a complete overview of the HEGABOX model performance we refer to [1].

It can be concluded that HGSYSTEM version 3.0 contains a model to simulate near-field dispersion of instantaneous releases, HEGABOX, which has a link to the far-field model HEGADAS-T. The results obtained with these models are in good agreement with experimental observations obtained at Thorney Island.

Error! Bookmark not defined.**.5. References**

1. Puttock, J.S., '*Comparison of Thorney Island data with predictions of HEGABOX / HEGADAS*', J. of Hazardous Materials, **16**, 439-455, 1987.

2. Puttock, J.S., '*A model for gravity-dominated dispersion of dense-gas clouds*', Stably stratified flow and dense gas dispersion, Conf. Proceedings, ed. J.S. Puttock, Clarendon Press, Oxford, 1988.