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A REVIEW OF MATHEMATICAL MODELS FOR THE ATMOSPHERIC DISPERSION OF HEAVY GASES. PART I. A CLASSIFICATION OF MODELS

PRZEGLĄD MODELI MATEMATYCZNYCH ROZPRZESTRZENIANIA SIĘ W ATMOSFERZE GAZÓW CIĘŻSZYCH OD POWIETRZA. CZĘŚĆ I. KLASYFIKACJA MODELI

Abstract: In this two part article in its first part models of heavy gas dispersion in the atmosphere are classified and the distinguished groups of models are characterised. In the second part the procedures for the model quality evaluation are described and the main results of model evaluation projects are summarised. Substances released to the atmosphere which have a density greater than the density of the atmospheric air are called heavy gases or dense gases. The dispersion of heavy gases is different from that encountered in the case of neutrally or positively buoyant gases. Specific models have been developed to describe it. The heavy gas dispersion models differ in the complexity and mathematical description. Based on these criteria four main groups of models are distinguished: simple/empirical models, intermediate/integral and shallow layer models, advanced/Lagrangian particle trajectory and Lagrangian puff dispersion models and sophisticated/Computer Fluid Dynamics (CFD) models. This classification is an extension of the classification proposed earlier in the literature.

Keywords: atmospheric dispersion, heavy gases, mathematical models

Introduction

The manufacture, storage, usage and transport of hazardous materials are a potential threat to people, environment and property. This has been shown in the past during the accidental releases of toxic or flammable or both substances. To minimise this threat special procedures have been established via international, European and national regulations as far as hazardous installations and transport of dangerous materials are concerned. These procedures include environmental impact assessment, safety studies, efficient land use planning and emergency response planning. In the implementation of these procedures the quantified description of the associated hazards is needed. This is called consequence assessment. For this purpose mathematical models have been developed. Since important

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decisions have to be made based on predictions of these models much attention has been paid to the evaluation of the models quality [1, 2].

In some accidental releases clouds which have a density greater than atmospheric air are produced. They are called heavy (or dense) gas clouds. The heavy gas cloud involves the gas which has a molecular weight greater then that of air (for example chlorine) or 'simulates' it due to one or several of the concurring reasons. The reasons are as follows: the low temperature of release (for example *Liquid Natural Gas*, LNG), high storage pressure and formation of aerosol following the release (for example ammonia), chemical reactions of the released substance with the water vapour contained in the atmosphere (for example hydrogen fluoride). The dispersion of heavy gas clouds differs from the dispersion of neutral or light gas clouds. The main differences include the additional gravity driven flow, wind shear at the interfaces, turbulence dumping and the inertia of the released material. In addition the formation of these clouds usually involves phase changes and heat transfer with the underlying surface [1, 3].

It is a common practice to divide the heavy gas cloud evolution into stages. For elevated releases the following stages can be distinguished: the emission from a source, airborne stage, touch down stage, gravity dominated (slumping) stage, transition stage and turbulence dominated (passive dispersion) stage. It is important to notice that during the cloud evolution not all the stages have to appear. For example the elevated heavy gas release can become passive sill before touching the ground. So there is no the gravity dominated stage and transition stage for this cloud. For ground level releases the airborne and touchdown stages are not present. To determine if density effects are important the dimensionless parameter such as the *Richardson number* (Ri) has been introduced. It depends on the density difference between the cloud and the atmospheric air, length scale (such as the cloud size or source dimension) and the characteristic turbulent velocity (such as the wind velocity, friction velocity or combination of the friction and convection velocities). As the specific definitions of Ri can be given in terms of different parameters the values of Ri are meaningful in relation to these definitions. The dispersion of the cloud is governed by the excess of density if the critical value of Ri is exceeded.

Mathematical models describing the behaviour of heavy gas clouds are called heavy (dense) gas dispersion models. The interest in the modelling of heavy gas dispersion goes back to the 1970s. The four decades of investigations have resulted in development of a great number of heavy gas dispersion models of different complexity and different approaches to the description of physical and chemical processes.

In this two part publication in the first paper a classification of heavy gas dispersion models and characteristics of the distinguished groups of models are presented. A list of publications on the comparisons of model results with measurements carried out by authors of models is included. They are usually presented in the same articles in which models are described. It is not claimed that the list is complete. In the second paper procedures for the quality evaluation of heavy gas dispersion models, main results of some evaluation exercises and databases containing the data from the heavy gas dispersion experiments are described [4]. This overview balances the historical achievements with the recent research in the field.

Classification of heavy gas dispersion models

General remarks

Mathematical models dedicated to the heavy gas dispersion differ in the completeness and methods of the description of physical and chemical processes taking place during the dispersion of heavy gas clouds, type of the release to which they apply, requirements concerning the input data, computer resources and computational costs, qualifications of the potential user [5]. Model capabilities and limitations influence their applications. Mathematical heavy gas dispersion models can be classified using different criteria. The model complexity or mathematical description are used as the criteria the most often. Based on these criteria heavy gas dispersion models are divided in this review into four main groups. They are given the following names: simple/empirical models, intermediate/integral and shallow layer models, advanced/Lagrangian particle trajectory and Lagrangian puff dispersion models, sophisticated/CFD models. This classification of heavy gas dispersion models can be treated as an extension of the classification proposed by the MEG (Major Evaluation Group) [6]. The MEG classification has distinguished three main groups of models which have been given the following names: phenomenological models, intermediate models, three dimensional models. In addition to some changes in the nomenclature the proposed classification introduces the main group of models named the advanced/Lagrangian particle trajectory and Lagrangian puff dispersion models. This division is implied in Koopman and Ermak [5]. The presented review takes also from earlier reviews of Britter [1, 7-9], Hanna and Drivas [3], Koopman and Ermak [5], Lees [10], Borysiewicz, Furtek and Potemski [11] and Markiewicz [12, 13].

It is worth mentioning that the presented classification of heavy gas dispersion models is an idealisation. Some models described in the literature seem not to fit neatly to any of the categories. There are also computer packages for which the term model is used which incorporate several modules of which each could be treated as an independent gas dispersion model. These model modules can form a sequence and the computer program automatically links the model modules required to trace the cloud. Each model module is treated separately in this classification. It seems important to notice here that in some earlier reviews [14, 15] the classification of heavy gas dispersion models opens a group called the modified Gaussian plume models. Models of this group illustrate the earliest attempts in the 1970s to simulate the heavy gas dispersion using the conventional Gaussian plume models developed for neutrally buoyant (passive) pollutants by modifying the values of dispersion parameters in the vertical direction. Examples of these models are described by Burgess and Zabetakis [16] and Clancey [17]. In the first model referred to as the Bureau of Mines model the Gaussian diffusion equation in the form presented by Pasquill-Gifford is used with the vertical dispersion coefficient σ_z being equal to $0.2\sigma_v$, where σ_v is the horizontal dispersion coefficient. In the model of Clancey the Gaussian diffusion equation in the form introduced by Sutton is used with the diffusion parameter in the vertical direction C_z taken to be half the value of the diffusion parameter in the crosswind (C_y) or downwind (C_x) directions $(C_y = C_x)$. This approach has come to be regarded as inadequate and it has been suppressed by other methods when experimental data has become available. This is why these models are not directly included in the proposed classification.

Table 1

Examples of heavy gas dispersion models and references on comparisons of model results with measurements carried out by authors of models

Empirical models (Model name or Model Authors names)

B and McQ [7, 8], VDI Guidelines [18]

Box models Van Ulden [20, 25, 27], Kaiser and Walker [21], DENZ [14], Eidsvik [23], Fay and Ranck [24], Fay and Zemba [26], Carpenter and coworkers [28], CIGALE [29], HEGABOX in HGSYSTEM computer package [54-56], GASTAR (GASeus Transport of Accidental Releases) for instantaneous releases [32], Cleaver and coworkers [33], Delvosalle and coworkers [34], DRIFT (*Dense Releases Involving Flammable and Toxics*) for instantaneous releases [35], Webber and coworkers [36], Kunsch and Fannelop [37], Nielsen [38], IIT (*Indian Institute of Technology*) I [39], Kunsch and Webber [40], Kumar and coworkers [41], UDM (*Unified Dispersion Model*) for instantaneous releases [136], UMDSAOS (*Uniwersalny Model Dyspersji Skazen w Atmosferze i Oceny Skutkow*, in Polish: Universal model of contaminant dispersion and consequences evaluation) for instantaneous releases [42]

Steady state plume models

Cox and Roe [50], Cox and Carpenter [51], Fay and Zemba [52], CRUNCH [53], Cleaver and coworkers [33], Delvosalle and coworkers [34], IIT II [39]

Generalised steady state plume models

HEGADAS (HEavy GAs Dispersion from Area Source) [54-56] in HGSYSTEM package, DEGADIS (DEns Gas DISpersion) [57], DRIFT for continuous releases [35], GASTAR for continuous releases [32], UDM for continuous releases [136], UMDSAOS for continuous releases [42]

One dimensional integral models

HMP (Hoot, Meroney and Peterka) [62], Ooms [61], Epstein [66], Edwards and Cleaver [65], AEROPLUME (*AEROsol PLUME*) and HFPLUME (*Hydrogen Fluoride PLUME*) in HGSYSTEM package [54-56], Khan and Abassi [68], a part of CLOUD (*Concentration Levels Of Unconfined Dispersion*) [69, 70], a part of UDM [63, 64], a part of UMDSAOS [42]

Shallow layer models

1D: Zeman [73], Meroney [75, 76], SLAB [74], DISPLAY-1 (*one dimensional shallow LAYer* model for DISPersion of heavy gas clouds) [77, 78], a part of CLOUD [69, 70]

2D: SLAM (Shallow LAyer Model) [79], TWODEE [80-84], DISPLAY-2 [85], Brambilla and coworkers [86, 87]

Lagrangian particle trajectory models

Schreurs [88], Gaffen [89], ADPIC (*Advection and Difussion Particle In Cell*) [90], Gopalakrioshnan [91], QUIC (*Quick Urban and Industrial Complex*)[92], Lee and coworkers [93], MicroSPRAY [94]

Lagrangian puff dispersion model

SCIPUFF (Second order Closure Integrated PUFF) [97]

RANS models

Specially dedicated codes: SIGMET [100, 101], TRANSLOCK [14], HEAVYGAS [102-104], FEM3 (*Finite Element Model*) [105-107], MARIAH [108], MERCURE-GL (mythological name-Gas de Lourd, in English: heavy gas) [109], Betts and Harountunian [110], ADREA-HF (*Atmospheriki Diaspora Rypwn* epi *Edafous Anomalon*, in Greek: the atmospheric dispersion of pollutant in irregular ground-*Heavy Fluid*) [111], MDPG (Modello per la Dispersione dei Gas Pesanti, in Italian: *Model of the dispersion of heavy gas*) [113], Pereira and Chen [114], Burman [115], Bayanov and coworkers [117], Ohba and coworkers [118], Scargiali and coworkers [119]

General purpose codes: FLACS (*FLame Acceleration Simulator*) [120-126], FLUENT [127, 128], CFX [129, 130], PHOENICS (*Parabolic, HyperbOlic and Elliptic Numerical Integration Code Series*) [136], STAR (*Simulation of Turbulent flow in Arbitrary Region*) [136], FDS (*Fire Dynamics Simulator*) [136]

LES models

Murakami and coworkers [132], Qiu and coworkers [131]

DNS models

Hortel, Michand and Stein [135], Cowan and Britter [134]

Simple/empirical models

In this group of models the dispersion of heavy gas clouds released to the atmosphere close to the ground is described by a series of nomograms or simple correlations [7, 18, 19]. They were created mainly at the end of the eighties based on the results of field or laboratory measurements limited to flat grassy terrain and neutral or slightly unstable conditions. The measured concentrations were averaged over the period of time of duration from 3 to 10 minutes. To derive the basic relationships the influence of atmospheric stability, surface roughness and averaging time was neglected. Instantaneous and continuous releases are distinguished. The centreline concentrations are calculated in terms of the following parameters: the gravity constant, downwind distance, density difference between the cloud and the atmospheric air relative to the atmospheric air density, heavy gas release volume or release rate, ambient wind velocity. Typical examples of these models are described in the Workbook on the dispersion of dense gases [7] and the German VDI Guidelines VDI 3783 [18]. The first model is referred to as the B and McQ model. It has been encapsulated in the TSCREEN (SCREENing Toxic air pollutant concentration) program. The second model has been imbedded in STOER (STOERfall, in German: accidental release) program. The VDI Guidelines model has been extended to non flat terrain with some geometric structures using the laboratory measurements carried out in 25 different configurations of street canyons, buildings or the intersections of basic geometric shapes [19]. These models should not be used for scenarios which are not closely related to the observations from which model relationships were derived. They are useful as screening tools. References on comparisons of model predictions and observations carried out by authors of models are given in Table 1.

Intermediate/integral and shallow layer models

In the second group of models, integral and shallow layer models can be distinguished. The integral models cover: box models, steady state plume models, generalised steady state plume models and one dimensional integral plume models. The shallow layer models are the most complex models in this group. This subdivision follows the MEG classification.

The box models are used to describe instantaneous releases with grounded clouds [20-44]. Pioneering ideas leading to their development were formulated in the mid seventies by van Ulden [20]. Mostly it is assumed that the pollution cloud forms a uniform cylinder with a specified size. The basic equations represent the cloud horizontal spreading, entrainment of the atmospheric air into the cloud and cloud heating. These ordinary differential equations are integrated with respect to time. The concentration averaged over the box volume is calculated knowing the mass of the substance released and the box volume. The box models allow for the different wind speed, surface roughness and atmospheric stability. The atmospheric stability is usually described using the Pasquill-Gifford stability classes. It is alternatively determined based on the Monin-Obukhov length. The cloud spreads in still air or is moved downwind at the velocity usually calculated based on the wind velocity. Alternatively the cloud velocity is determined based on entrained momentum. The horizontal spreading influencing its radius is assessed using a gravitational front velocity. It calculated based on the gravity current formula:

$$u_{f} = K\{g[(\rho_{c} - \rho_{a})/\rho_{a}]h\}^{0.5}$$
(1)

where: *K* is the coefficient with the value close to unity, *g* is the gravitational constant $[m s^{-2}]$, ρ_a and ρ_c are the densities of the atmospheric air and cloud $[kg m^{-3}]$, *h* is the height of the cloud [m]. The exchange of the mass between the cloud and the atmospheric air taking place through the top and edge of the cylinder leading to the cloud diffusion is described by entrance velocities. The values of these parameters are calculated based on empirical formulas. They differ for the top and the edge. The edge entrainment velocity is usually scaled with the front velocity. However in some models the edge entrainment is neglected. For the top entrainment velocity various formulas are used. They are generally of the form:

$$u_{e,t} = u_t f(Ri) \tag{2}$$

where: u_t is the characteristic turbulent velocity [m s⁻¹], *f* is a function of the local cloud Richardson number Ri [-]. The friction velocity or combination of the friction velocity and convection velocity are usually used as a characteristic velocity. The function *f* usually has the form:

$$f = a/(1+bRi) \tag{3}$$

where: a and b are empirical constants. Alternative parameterisations for the front velocity and top entrainment velocity have been proposed by van Ulden [25]. They are obtained from the radial momentum budget and bulk turbulent kinetic energy budget, respectively. The cloud heating being the result of its contact with the ground and cloud dilution by the atmospheric air are introduced straightforwardly. In some models unsteady heat transfer effects are simulated. In more refined box models also other thermodynamic effects such as the phase changes of the released material and the water vapour are considered. The thermodynamic modules are usually based on the assumption of homogenous equilibrium [45, 46]. Some thermodynamic modules can describe basic chemical reactions for specific substances such as hydrogen fluoride or ammonia with water in moist air. In the neutrally buoyant phase the dispersion is usually described using the classical Gaussian equation for a puff. The concept of a virtual source is used to calculate the dispersion coefficients at the transition point. To determine when the transition to neutrally buoyant dispersion occurs usually the following alternative criteria are used. The first test is based on the difference of densities between the cloud and the atmospheric air. The second test compares the growth of the cloud radius due to gravitational slumping to the one expected from atmospheric turbulence and the entrainment top velocity to the atmospheric turbulent velocity. The variation of concentration in the box can be later introduced by assuming empirical similarity profiles in the vertical or horizontal direction and dependence on the cloud dimensions. In more refined box models the transition from heavy gas to passive dispersion is smooth and the fairly general profiles for concentration in the vertical and horizontal directions are assumed which comprehend among others the top hat profile and the Gaussian profile. The profiles evolve in time. The significance of this is that it allows to write equations for bulk quantities all the way into the passive regime without the need for any discontinuity in the approach. The horizontal concentration profile parameter depends on the normalised density differences between the cloud and the atmospheric air. The vertical concentration profile parameter is extracted from the turbulent diffusivity profile. Flat uniform terrain is assumed in most of box models. In only some of these models the dispersion on slopes or over fences and simple obstacles is described. The box models satisfactorily reproduce many aspects of field and laboratory experiments. The empiricism in these and other integral models has a clear physical interpretation. Input data needed by these models are easy to obtain, computing costs are low or reasonable. The same concerns the requirements concerning computer resources and potential user qualifications. These features make the box models and other integral models valuable engineering tools. They are used for environmental impact assessment, risk assessment, emergency response planning and efficient land use planning [47-49]. Examples of box models are presented in Table 1.

The steady state plume models are used for continuous grounded releases [33, 34, 39, 50-53]. The first models of this group were created in the late seventies. They are developed in a similar manner as the box models. All basic phenomena associated with dense gas releases such as the horizontal spreading, exchange of mass between the plume and the surrounding air, plume heating are described by ordinary differential equations. However, here these equations are usually integrated with respect to the downwind distance. The plume cross section is assumed to be a rectangle. The plume properties are averaged over the plume cross-section. The average concentration is calculated knowing the mass flow rate of the substance and the volume flow rate of the plume. The meteorological information required in these models is the same as in the box models. It usually covers standard data: the wind velocity at specific height, stability of the atmosphere, air and ground surface temperature, atmospheric pressure and air ambient relative humidity. It is generally assumed that the terrain is flat and the surface roughness is the only one parameter needed to describe the terrain. The plume moves downwind with the velocity usually calculated based on the wind velocity. Alternatively the plume velocity is calculated from the momentum equation. The models are capable to treat only the basic thermodynamic effects as the simple box models do. The Gaussian or other simple similarity profile can be later adjusted for concentrations. The edge and the top entrainment velocities are typically calculated from the same relationships as in the box models. The horizontal spreading is given by the gravity current formula. The criteria for transition to the passive plume dispersion are again taken from the early box models. The passive plume dispersion in the far field is described by the Gaussian plume formula using the dispersion coefficients for passive releases. Only in some models the dispersion over fences and simple obstacles is described. Examples of models are given in Table 1.

The generalised steady state plume models [32, 35, 42, 54-60] can be considered as an extension of the steady plume models in the sense that the spatial variation of concentrations and other parameters in the plume cross-section follow fairly general similarity profiles which change as the plume travels downwind. This assures continuity as the heavy plume becomes passive and allows us to describe the physical processes in the far field with the same approach without the need to define a transition point and the use of separate models for different regimes. The HAGADAS (*HeAvy GAs Dispersion from Area Sources*) model included into the HGSYSTEM computer package [54-56] and the DEGADIS (*DEns GAs DISpersion*) model [57] are the most popular examples of the models of this group. The HEGADAS model has been formulated by the gradual developments [58, 59] of the model originally described by te Riele [60]. The DEGADIS model in turn has been developed based on HEGADAS. It is encapsulated into ALOHA (*Aerial LOcation of Hazardous*)

Atmospheres) program which in turn is a component of CAMEO (Computer Aided Management and Emergency Operations). In these models the plume cross-section is a rectangle. The concentration profile in the vertical direction is Gaussian but in the horizontal crosswind direction it has Gaussian features at the edges. The horizontal crosswind profile is uniform in the middle part of the plume and becomes fully Gaussian when the middle flat part disappears. In other generalised steady state models the plume cross-section is usually elliptical and the profile for concentrations smoothly changes from top hat to Gaussian along the plume path. They are capable to deal with thermodynamic effects at the same level of details as the refined box models. The same concerns other features such as chemical reactions or description of meteorological conditions. Their requirements concerning input data, computer resources and qualifications of potential users are also similar to those in the refined box models. Examples of models are given in Table 1.

The one dimensional integral plume models are used to describe continuous, elevated releases [61-72]. The pioneering work in the simulation of this phenomenon was done in the mid-seventies by Ooms [61] and Hoot, Meroney and Peterka [62]. The models of this group are based on the conservation equations of the mass, species, downwind and crosswind momentum and energy averaged over the plume cross-section. These equations directly predict plume variables averaged over the plume cross-section. The cross-section of the plume is assumed to be a circle, ellipse or rectangle. A uniform, Gaussian or generalised shape similarity profile is used to describe the space variability of plume variables in the cross-section of the plume while averaging plume variables over the plume cross-section to simplify the equations. The same profiles can be later used to reintroduce spatial variability of these variables. In the steady state models the plume variables are evaluated along the plume trajectory. In time dependent models the plume variables change along the plume trajectory and in time. The elevated release may become the passive elevated plume in the far field or may touch the ground still being sufficiently dense. In the first case it is treated as the elevated passive plume. In the second case after touching the ground it can be linked to the ground level heavy gas dispersion model. The gravity, drag force of the ambient flow and momentum of the entrained air influence the elevated plume path. The entrainment velocity in these models is different from that for the models of grounded clouds. It is composed of several terms corresponding to different mechanisms. The jet turbulence, cross-flow perpendicular to the plume axis and atmospheric turbulence are usually taken into account. The contribution due to the jet turbulence is typically determined from the formula [71]:

$$u_{e,i} = c_1 |u_c - u_a \cos \theta| \tag{4}$$

where: u_c is the mean or centreline plume velocity (they are equal for top hat profile), u_a is the wind velocity, θ is the angle between the plume centreline and the horizontal axis, c_1 is the empirical constant. In some models the right side of the formula is multiplied by $(\rho_c / \rho_a)^{1/2}$. The contribution due to cross flow perpendicular to the plume axis is usually calculated with the formula [71]:

$$u_{e,c} = c_2 |u_a \sin \theta| \tag{5}$$

where c_2 is the empirical constant. In some models the right side of the formula is multiplied by $|\cos\theta|$. Different methods are used to describe the contribution due to atmospheric turbulence in the near field (close to the source). In some models it is neglected. In other models it is either derived from the relations for dispersion coefficients from the conventional Gaussian plume formula or it is described using the method proposed by Ooms [61]:

$$u_{e,nf} = c_3 u' \tag{6}$$

where: u' is the relevant atmospheric turbulence intensity, c_3 is the empirical constant. Some authors use the friction velocity instead of u'. The test to determine when the elevated heavy gas dispersion changes into elevated passive dispersion often includes the following criteria. The plume velocity is close to the ambient wind velocity. The total entrainment of air to the plume is close to the entrainment corresponding to the atmospheric turbulence. The input data required by these models is similar to the ones required by other integral models. The same concerns thermodynamic effects and chemical reactions. However for the airborne plume the heating from the ground is not considered. Reviews of models have been given by Ooms and Duijum [72] and by Bricard and Friedel [71]. Examples of models are given in Table 1.

The one or two dimensional shallow layer models are used for grounded releases [73-87]. The foundation to this group of heavy gas dispersion models was given in early eighties by Zeman [73]. These models are based on partial differential equations describing the principles of conservation of the mass, species, momentum and energy. In two dimensional models these equations are averaged over the cloud depth. This kind of averaging is convenient due to the geometry of the cloud. Its vertical dimension is small compared with its horizontal dimensions. In one dimensional models the model equation are averaged over the cloud cross-section. In general as a first approach uniform profiles are assumed to describe the plume variables while averaging the conservation equations. Approximations of the shallow layer theory state that the pressure distribution is hydrostatic. In some models it is assumed that this approximation is valid for the entire cloud. In other models it is kept within the main body of the cloud and the dispensation is made only for the special processes at the leading edge. Different approaches have been proposed to allow for non-hydrostatic pressure in the front and to enforce constant Froude number coupled with the shallow layer model. In the first method the front is treated as discontinuity and its velocity is calculated as in the ground level integral models using the gravity current formula. This method requires to keep track of the front footprint. It is easy to implement in the one-dimensional models in which the discontinuity is a point but it is not trivial in two-dimensional models in which the discontinuity is a line. So in practice this method has been used only for one-dimensional models and has not been extended to two-dimensional models. An alternative second method is to add the new terms to the water equations which become active near the fronts. These new terms account for the interaction between the ambient fluid and the dense layer. They simulate the backward force exerted on the dense layer by the ambient fluid by virtue of its motion. The force is small everywhere except near the leading edge and it is of the correct magnitude to ensure that the leading edge advances at a constant front Froude number. In this manner the front Froude number may be fixed. This method has been used in one- and two-dimensional models. It seems important to notice that there is no agreement how to treat the leading edge in the shallow layer models. Some authors have reported that the implementation of these methods reveals waves in the following flow. In the shallow layer models the exchange of the mass between the pollutant cloud and the atmospheric air is described usually by the entrainment velocity. There are however some exceptions. In the SLAM (Shallow LAyer Model) model [79] it is assumed that the pressure is non-hydrostatic and the entrainment rate is estimated based on the local turbulent kinetic energy which is calculated explicitly from the balance equation. In shallow layer models conservation principles are used to treat the effects of gravity such as slumping or down slope transport. Some terms are added to the momentum equation. This is an advantage in comparison with the integral models, which in general, are not suitable for complex topography. The treatment of fences or buildings is not easy in the shallow layer models. Only some models include the influence of fences or buildings on the cloud dispersion. The shallow layer models do not account for the passive dispersion. There is no obvious method to simulate this phenomenon in these models. Most of the shallow layer models are limited to one phase releases. They usually treat the effects of ground heating of the cloud. The ambient flow outside the cloud is usually described based on the standard meteorological data from a single point as in the integral models. However it is possible to supply to the shallow layer models the ambient flow specified at each point in space running the three dimensional prognostic or diagnostic meteorological model prior to shallow layer simulations. The shallow layer models allow for a realistic description of the behaviour of the heavy gas clouds in the flat or sloping terrain. The two dimensional shallow layer models possess a combination of advantages and disadvantages of integral and RANS models which belong to the CFD models. They are less empirical than integral models and more easily used than RANS (Reynolds Averaged Navier Stocks equations) models. The time to run them is somewhere between the time to run these two types of models. These models have a potential to be routinely used in consequence assessment especially in sloping terrain however no information in the literature has been found to confirm that any model of this group has moved from the status of the research to the engineering tool. Examples of models are given in Table 1.

Advanced/Lagrangian particle trajectory and Lagrangian puff models

The Lagrangian particle trajectory models for heavy gas dispersion have been derived from the codes for neutrally buoyant pollutants [88-94]. They generally can treat both elevated and ground level releases however most of early models built at the end of the eighties or in the early nineties take into account either elevated or ground level releases. In the models of this group the mass of the released heavy gas is represented by pseudo-particles. The transport and dispersion is simulated following the trajectories of these particles. A displacement of the particle during the time step is obtained by adding up the effects of the mean flow (wind), atmospheric turbulence and excess of density. The mean usually three dimensional wind field is provided as an input to the Lagrangian particle trajectory model. It is obtained from a separate prognostic or diagnostic meteorological model. The meteorological models have been described among others in Markiewicz [95, 96]. The turbulent velocities are obtained solving the three dimensional form of the Langevin equation. The turbulent flow properties (characteristics) such as the turbulent kinetic energy and its rate of dissipation or the variance of the wind velocity and Lagrangian time scales are issued from the meteorological model. Reductions of the values of these turbulence quantities due to negative buoyancy of heavy gas clouds are expressed in terms of the local gradient Richardson number or density difference between the particles and the air. As far as the excess density effects are concerned they are different for elevated and ground level heavy gas clouds. In case of elevated releases excess density effects cover the vertical downward acceleration of particles. In case of ground level clouds horizontal spreading and vertical slumping has to be described. An inclusion of these effects in Lagrangian particle trajectory models is not trivial because it requires to link the transport of individual particles to the collective behaviour of all particles. In the early models for elevated releases without momentum the vertical acceleration of the descending particle is estimated by considering the buoyancy and gravity forces acting on a particle. In the modern models for the elevated plumes with or without momentum the particle trajectory is estimated solving a set of equations describing the conservation of the mass, energy, vertical momentum and two horizontal momenta. The horizontal spreading of the grounded cloud is estimated either by simple algorithms derived from the gravity current formula, in which the column integrated density is used or by two dimensional flow models developed based on the shallow layer theory, in which the cloud properties in the vertical direction are averaged. The slumping velocity is then obtained from the continuity equation (assuming the non-divergence condition) or it is taken to be proportional to the local difference in column integrated densities. When the cloud is diluted enough to approach the neutrally buoyant dispersion a smooth transition is obtained since the same Lagrangian particle trajectory model continues to be used without gravity effects added. At present any of the Lagrangian particle trajectory models account for thermodynamic processes except the ADPIC (Advection and Diffusion Particle In Cell) model [90] which takes into account only heating from the ground. The solution of this problem is not simple. The models are able to take into account complex terrain (realistic topography and obstacles). They are generally run in conjunction with three dimensional prognostic or diagnostic meteorological models. The Lagrangian particle trajectory models can be placed somewhere between the integral and RANS models as far as their demands are concerned. These models coupled especially with the diagnostic meteorological models are well suited for routine uses for the preparedness purpose in complex terrain due to their robustness and relatively high computational speed. Examples of models are given in Table 1.

There is one Lagrangian puff dispersion model to simulate the dispersion of heavy gas releases of different type [97]. It has been derived from the SCIPUFF (*Second-order Closure Integrated PUFF*) code for neutrally buoyant pollution. It uses a Gaussian puff to describe the concentration field as a sum of contributions from the collection of puffs. It can use different types of meteorological data including the three dimensional gridded data. The fluctuation terms due to ambient atmospheric turbulence are parameterised using the second closure model of Donaldson and Lewellen [98, 99]. The original model for passive pollution has been extended to cover dynamical effects due to puff buoyancy and the reduction of vertical turbulent diffusion. Negatively buoyant puffs remote from the surface simply fall downward under the buoyancy forcing. For the puffs that interact with the ground surface the effects associated with the dense gas slumping on the ground are represented by lateral divergence of the velocity field with a magnitude based on conservation of the moment of vorticity. The reduction of vertical turbulent diffusion to some provide the sumple dense cloud and the ambient turbulent motions. The turbulent entrainment model for a dense gas cloud which interacts

with the ground uses the estimates of the internal velocity scale of the puff and the length scales appropriate for a stably stratified dense cloud. The ambient vertical eddy diffusivity and puff centroid velocity are calculated using the dumping factor the value of which depends on the puff Richardson number. The model does not treat the thermodynamic effects. The model predictions have been compared with the experimental data.

Sophisticated/CFD models

The CFD models are three dimensional models in which a full set of partial differential equations dependent on time and three space coordinates describing the principles of conservation of the substance, mass, momentum and energy are solved. These models can be applied to any type of emission scenario, terrain and meteorological conditions. The conservation principles are used to treat the effects of gravity. The description of the physical processes of the heavy gas dispersion is detailed and complete. The models can be divided into three groups depending on the form of equations used: RANS models, LES (*Large Eddy Simulation*) models and DNS (*Direct Numerical Simulation*) models. This subdivision is implied in Britter [9].

Most of CFD codes capable to handle the heavy gas dispersion are RANS models [100-130]. They appeared in the field of heavy gas dispersion in the late 1970s. The RANS models solve the equations for the mean properties of the flow (the Navier Stocks equations which express the conservation of momentum together with the mass, energy and substance conservation equations) and assume turbulence modelling with the turbulence closure model. To simplify the model equations the hydrostatic, anelastic or Boussinesq approximations are introduced. The methods of solution of equations include the *finite* difference methods (FDM), finite element methods (FEM) or finite volume methods (FVM). Particular attention in RANS models is paid to the turbulence modelling. In the earlier RANS models the turbulence modelling has been based on the K theory closure but nowdays it is usually based on the k- ε closure. However the other closure models such as the k-l closure, k-\u00f8 closure, SST (Shear Stress Transport) closure and SSG (Speziale Sarkar *Gatski*) closure have been also tested. It seems important to notice that all turbulence models require empirically determined coefficients. This is also true for the subgrid turbulence models in LES models. In this respect turbulence models share the commonality of invoking empiricisms with the integral models however they differ significantly by degree. The turbulence closure model based on the K theory assumes local equilibrium and uses diffusion coefficients that depends on the local properties of the cloud and the ambient atmosphere. It is based on the Richardson number. The other mentioned turbulence closure models do not assume the local equilibrium and allow for the creation, transport and dissipation of turbulence. The k- ε turbulence closure belongs to the family of eddy viscosity closures. It introduces two new variables into the system of conservation equations. These variables are the turbulent kinetic energy (k) and the turbulence dissipation rate (ε). These variables are directly calculated from the differential transport equations for the turbulence kinetic energy and turbulence dissipation rate. It is assumed that the turbulence viscosity is a function of the turbulence kinetic energy and the turbulence dissipation rate. This closure type has proven to be stable and numerically robust having the well established predictive capability. The k-l turbulence closure is also a kind of the eddy viscosity closure. The turbulent viscosity is assumed to be a function of the turbulent kinetic energy (k) and a turbulent length scale (l). The turbulent kinetic energy is found by solving a conservation equation where one of the most important terms is the turbulent energy dissipation. The dissipation is assumed to be a function of the turbulence kinetic energy and the length scale. The k- ω closure belongs to the eddy dissipation models. In the k- ω closure the turbulence viscosity is linked to the turbulent kinetic energy and the turbulent frequency (ω). These two variables are determined from the turbulence kinetic energy conservation equation and the turbulent frequency conservation equation. The SST closure is also the eddy dissipation model. It has been developed to remove a deficiency of both the k- ε and k- ω turbulence closures which do not account for the transport of the turbulent shear stress resulting in the over prediction of the eddy viscosity. It is based on the same equations as the k- ω closure but in addition a limiter to the formulation of the eddy viscosity is introduced. The Reynolds stress model is based on transport equations for all components of the Reynolds stress tensor and the dissipation rate. These turbulence models are generally flexible but the increased number of transport equations leads to a higher degree of complexity, reduced robustness and increased computational costs. The results of simulations carried out with the MERCURE-GL (mythological name-Gas de Lourd, in French: heavy gas) and ADREA-HF (Atmospheriki Diaspora Rypwn epi Edafous Anomalon, in Greek: the atmospheric dispersion of pollutants in irregular ground-Heavy Fluids) models indicate that both the k- ε and k-l turbulence closure are capable to reproduce the heavy cloud behaviour sufficiently well to simulate realistic concentration fields [116]. The results of the simulations carried out by Sklavounos and Rigas [124] based on the CFX code with the four turbulent closure modules SSG, $k - \varepsilon$, $k - \omega$ and SST show good agreement compared with the experimental data. The k- ω and SST models show improved robustness. The SSG model entails increased CPU time without significant enhancement of accuracy of results. The SSG, k- ε and SST models appear to overestimate maximal concentrations recorded in the trials, whereas the k- ω model underestimates them. The examples of RANS models are given in Table 1. The special purpose models developed specially for heavy gas dispersion and general purpose commercial codes applied in this field are included. Obviously a general purpose CFD code can not be applied straightforwardly in a problem but only constitute the basis on which an appropriate numerical model will be built. The RANS models represent a good compromise between results accuracy and computational efforts. They have a potential to be used in post accidental consequence assessment for a complex scenario. However it is unlikely that they will be used for a very large number of scenarios due to the high degree of expertise and labour demands, the high software purchase costs and the large computational costs required. However if the local topography is very complex they can be the only practical option.

The LES models solve the equation for the mean flow and for the large eddies and assume turbulence modelling at the small scales [131, 132]. The Smagorinsky turbulence closure [133] or some modification of this turbulence model is used. The simulations of heavy gas cloud dispersion using the LES models are described by Murakami, Mochida and Tominaga [132] and Qiu, Guo and Lin [131]. An application of the LES models in solving practical tasks is questionable mainly due to high computer costs, input data requirements and labour intensity. They are rather used as research tools to improve understanding of the process and to provide direction for the improvement of less computationally expensive models.

DNS models solve the exact equations with fine meshes and time steps without the assumption of turbulent closure [134, 135]. They are computationally intensive and currently only practicable for simple flows at low Reynolds numbers. The DNS used for heavy gas dispersion is described by Hortel, Michand and Stein [135]. Also Britter and Cowan [134] used DNS for simulation of gravity currents. The DNS codes are extremely demanding in technical issues and expertise. They are only used as research tools for specific cases. Usually simulations are carried out parallel with the experimental investigations of the process.

Conclusions

The heavy gas dispersion models can be divided into four groups: simple/empirical models, intermediate/integral and shallow layer models, advanced/Lagrangian particle and Lagrangian Gaussian puff models, sophisticated/CFD models. In the group of integral models four subgroups are distinguished: box models, steady state plume models, generalised steady state plume models and one dimensional integral plume models. The CFD models include: RANS models, LES models and DNS models. The models of the first three main groups and RANS models are engineering tools or have a potential to become so. The other CFD models are research models. The progress in heavy gas dispersion modelling within the last decade concerns mainly the RANS models. In particular attention has been focused on development and testing of the new turbulence closure models and application of the commercial general purpose codes. Also a renewed interest in the Lagrangian particle trajectory models and shallow layer models needs to be noticed. In the shallow layer models a new approach to the treatment of the front propagation has been proposed. In the Lagrangian particle trajectory models new methods to describe the excess density effects have been introduced.

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PRZEGLĄD MATEMATYCZNYCH MODELI ROZPRZESTRZENIANIA SIĘ W ATMOSFERZE GAZÓW CIĘŻSZYCH OD POWIETRZA. CZĘŚĆ I. KLASYFIKACJA MODELI

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Abstrakt: W tym dwuczęściowym artykule w pierwszej części dokonano klasyfikacji modeli rozprzestrzeniania się w atmosferze gazów cięższych od powietrza i scharakteryzowano wyróżnione grupy. Gazami cięższymi od powietrza nazywa się te substancje emitowane do atmosfery, których gęstość jest większa od gęstości powietrza. Rozprzestrzenianie się w atmosferze gazów cięższych od powietrza różni się od rozprzestrzeniania się gazów o gęstości mniejszej od gęstości powietrza. Do opisu tego zjawiska opracowano specyficzne modele. Modele rozprzestrzeniania się gazów cięższych od powietrza różni się od powietrza różnią się stopniem skomplikowania i sposobem opisu matematycznego. Wykorzystując te dwa kryteria, można wyróżnić cztery grupy modeli: proste/empiryczne modele, pośrednie/zintegrowane i płytkiej warstwy modele, zaawansowane/ Lagrange'owski trajektoryjne modele cząstek i Lagrange'owski modele obłoku, skomplikowane/modele komputerowe dynamiki płynów. Klasyfikacja ta jest rozszerzeniem klasyfikacji proponowanej już w literaturze.

Słowa kluczowe: rozprzestrzenianie się zanieczyszczeń w atmosferze, gazy cięższe od powietrza, modele matematyczne