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# MATHEMATICAL MODELING OF HEAVY GAS ATMOSPHERIC DISPERSION OVER COMPLEX AND OBSTRUCTED TERRAIN

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Abstract: In this article the capabilities of mathematical heavy gas atmospheric dispersion models to describe the dispersion of heavy gases in complex and obstructed terrain are presented. The models have been categorized into three main classes: phenomenological (empirical) models, intermediate (engineering) models and computational fluid dynamic (research) models. Each group of models is discussed separately. The general features of the models are discussed briefly. Examples of the heavy gas atmospheric dispersion models capable to treat the influence of non-flat and obstructed terrain on the heavy gas dispersion result from the work carried out in the European Union and in the US. No model simulating the heavy gas atmospheric dispersion over complex or obstructed terrain has been yet developed in Poland. The need for future work on the effects of complex and obstructed terrain on the heavy gas atmospheric dispersion is expressed. Future research in the area should include both experimental and modeling work. In the context of this paper future modeling work is worth considering in more detail. It seems that all the approaches to describe the heavy gas atmospheric dispersion over complex and obstructed terrain are worth further attention. This opinion is supported by the fact that these approaches are used in different types of heavy gas dispersion models, which in turn differ in applications. The simpler methods are introduced to the simpler heavy gas atmospheric dispersion models applied mainly in the routine calculations. The advanced techniques capable to describe the flow near complicated geometries are used in the sophisticated models applied mainly as a research tools.

# INTRODUCTION

The dispersion of heavy gases (dense gases or negatively buoyant gases) in the atmosphere differs considerably from the dispersion of passive gases (neutrally buoyant gases) and light gases (positively buoyant gases). The main phenomena particular to heavy gases are: the alternation in turbulent diffusion, gravity flow and, for cold gases, the effects of the heat flow from the ground to the cloud. The heavy gas cloud evolution can be divided into several phases: the source emission phase, internal buoyancy dominated phase, transition phase and passive dispersion phase (the ambient turbulence dominated phase). Heavy gases form low-level clouds that are sensitive to the effects of topography and obstructions. A heavy gas can be denser than air for a number of reasons:

- its molecular weight is greater than that of air (e.g. chlorine);
- it is significantly colder than air (e.g. cold methane evolving from the refrigerated liquefied natural gas (LNG) spilled on the ground);

- it consists in part of aerosol particles (i.e. ammonia);
- it reacts with water vapor in the air (e.g. nitrogen tetroxide, hydrogen fluoride).

Special heavy gas atmospheric dispersion models have been developed to treat the heavy gas dispersion in the atmosphere. These models differ considerably in their physical completeness, numerical complexity, computational costs, input data requirements, width of applicability and ease of use. The models can be categorized into three main classes [28, 32]: phenomenological (empirical) models, intermediate (engineering) models and computational fluid dynamic (research) models.

This article presents the capabilities of heavy gas dispersion atmospheric models to describe the atmospheric dispersion of heavy gases over complex and obstructed terrain. The general features of the models are discussed briefly. These are given in other publications [6, 28, 32, 37]. The attention is focused on the heavy gas dispersion model characteristics concerning the dispersion in complex and obstructed terrain. Examples of the models result from the work carried out abroad, mainly in the European Union and in the US. No model simulating the heavy gas atmospheric dispersion over complex or obstructed terrain has been yet developed in Poland. The need for the future work is expressed and some tasks are formulated.

# APPROACHES TO DESCRIBE THE EFFECTS OF COMPLEX AND OBSTRUCT-ED TERRAIN ON THE DISPERSION OF HEAVY GASES IN THE ATMOSPHERE USED IN MATHEMATICAL MODELS

#### Phenomenological models

Phenomenological models are the simplest class of all the heavy gas atmospheric dispersion models. They are used as screening tools. 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 derived from the analysis of empirical data. Instantaneous and continuous releases are distinguished. The centerline ground level concentration of the heavy gas is calculated as a function of a downwind distance in terms of the gravity constant, density difference between the gas and the ambient air, release volume or release flow rate, ambient wind velocity. The basic relations to calculate concentrations refer to the conditions that ignore the effects of topography and obstacles.

The phenomenological models cannot account for the effects of complex and obstructed terrain in general. However, extension of these models for the treatment of simple topographical features and single obstacles is possible using the empirical approach. The parameters of heavy gas clouds interacting with these obstructions are described by simple relations derived from the analysis of observations of the heavy gas released in such conditions. Examples of these models are described in the Workbook on the dispersion of dense gases [4] and the German VDI (Verein Deutscher Ingenieure) Guidelines Part II [50]. In the Workbook [4] the treatment of complex topography is considered by introducing two limiting cases:

- the topographical feature is large compared to the scale of a released heavy gas volume and then topography reduces to a local slope;
- the cloud is very wide compared to the topographic feature and then the heavy gas may flow around (or over) the topography and be diluted in a wake of the topo-

graphic feature.

For the treatment of the effects of buildings and obstacles also two cases are discussed:

- the release is upwind of the fence;
- the release is in the immediate lee of the building.

The procedures from the Workbook are coded as part of the TSCREEN (SCREENing Toxic air pollution concentrations) program [49]. The VDI guidelines [50] have extended the work to include the effects of obstacles on the plume behavior including street canyons, buildings, or the intersection of basic geometrical shapes for a total of 25 different configurations. The procedures from VDI Guidelines Part II are coded as part of the STOER (STOERfall: in German, an accidental release) program [12].

### Intermediate models

Models in this group are intermediate in complexity between computational fluid dynamic models and phenomenological models. They are used in routine calculations. The group of intermediate models can be further divided into the following subgroups: box models, steady state plume models, generalized steady state plume models, one dimensional integral plume models and shallow layer models.

Box models are used to describe instantaneous releases with grounded clouds. The cloud in a flat and open terrain is simplified to a uniform, widening cylinder. The cloud's properties are averaged over the cloud's volume. The basic equations used in these models represent the cloud's horizontal spreading, mass and energy conservation. In these ordinary differential equations time is the independent variable. The horizontal spreading is assessed using a front velocity. The exchange of the mass between the cloud and the atmospheric air taking place through a top and an edge of the cylinder is described by entrainment velocities. The cloud spreads in still air or moves downwind with the velocity dependent on the wind velocity. The variation of concentration in the box volume can be reintroduced assuming empirical similarity profiles in the vertical and horizontal directions.

Extension of the box models to complex and obstructed terrain is not possible in general. However, there are modifications of the conventional box models for simple cases of non-flat and obstructed terrain in which it is assumed that the cloud retains its form. Modifications cover the following problems:

- simple slopes;
- valleys with a uniform cross section;
- simple obstacles such as fences and buildings.

The influence of simple slopes on heavy gas dispersion has been considered, for example in the works of Kukkonen and Nikimo [25] and Webber *et al.* [56], Tickle [48] and Ross *et al.* [41]. In the model of Kukkonen and Nikimo [25] the cloud advection is described from the balance of gravitational and drag forces for a bulk cloud. The influence of sloping ground on the spreading and dilution of the cloud is neglected. The model allows for any angle between the incline and the wind direction. The released gas keeps the form of a uniform cylinder. The behavior of the heavy gas clouds moving down the slope is complicated and this last assumption seems unrealistic.

Webber *et al.* [56] have presented a model in which for the release on a uniform slope, without wind, surface friction or entrainment the wedge shaped cloud is formed.

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The cloud has a horizontal upper surface, a front of universal shape and a rear boundary which intersects the terrain. This cloud geometry is based on the observations of a solution from the shallow water equations on a slope with specific boundary conditions. In this model the cloud motion down a slope is a result of the balance of gravity and air resistance at the front. The comparisons with wind tunnel data in Webber *et al.* [56] have shown that the predicted cloud velocity becomes too fast for steep slopes.

Tickle [48] has refined the wedge shaped model of Webber to include the dilution of the cloud. The dilution is modeled assuming that the entrainment is directly proportional to the down slope advection. The model parameters are the entrainment coefficient and a frontal Froude number and values for these have been determined by being fitted to the experimental data of Schatzmann [44]. The predictions of the Tickle's model appear to be broadly consistent with the experimental data of Schatzmann [44] and Flacher *et al.* [15].

Ross *et al.* [41] have developed a model in which the cloud shape is not restricted to the shape prescribed by the wedge model of Webber, but can be used for any self-similar shaped wedge. In this model the down slope motion of the cloud is due to two main forces: the buoyancy force and the drag force associated with the motion. The drag force is made of the bottom drag and the form drag. The form drag is equivalent to imposing a Froude number condition on the front, as done by Webber *et al.* [56] and Tickle [48]. The entrainment coefficient has been determined by being fitted to experimental data and has been found to depend very little on the slope. Ross *et al.* [41] have tested and compared three wedge models with their experimental data. However, in predictions their model is more successful than the other two models none of the three simple wedge models capture all the significant features of the flow. In the models the current takes the form of a more complicated current. Nielsen [38] has extended the analytical wedge shaped model of Webber to a v-shaped valley. In addition he gives a numerical solution for a parabolic shaped valley.

As far as the simple obstacles are concerned their influence on the heavy gas dispersion is considered in the works of Cleaver *et al.* [10] and Webber *et al.* [57]. Cleaver *et al.* [10] have combined separate empirical algorithms for the effects of fences and idealized buildings on heavy gas dispersion derived by Britter [5] into a single algorithm and they have implemented it to a conventional heavy gas dispersion model for flat and unobstructed terrain. This enables predictions to be made for dispersion over a typical industrial site in which obstructions do not divide neatly into fences or isolated buildings. Porous obstacles are treated by the introduction of a solidity factor. The value of it is equal to the fraction of the frontal area that blocks the path of the advecting cloud. For a group of buildings it is assumed that:

- if the spacing between obstacles is large (larger than two buildings heights), the effect of the group of obstacles is equivalent to the linear superposition of the effects of individual obstacles considered in isolation;
- if the spacing between obstacles is small, the sheltering of the building downstream by the upstream building is taken into account by using a reduced solidity factor, whose value is directly proportional to the fraction of the frontal area that is sheltered by the upstream building.

Britter [5] has based his analysis on his observations of the behavior of the steady heavy gas plumes interacting with a fence. He argues in particular that:

- if the plume height is low when it crosses the fence then the plume increases in width upstream of the fence and dilutes in the lee;
- if the plume height is large compared to the fence height then its effect is negligible;
- and in the analysis the two quantities of primary importance are cloud Richardson number and a ratio of the fence height to the plume height.

Britter [5], deriving the empirical algorithms assumes that the conditions upstream of an obstacle are unaffected by its presence. In this way single discontinuity is introduced in the calculated cloud variables to account for the complex changes that occur in reality as the cloud interacts with an obstacle. The algorithms predict the conditions immediately downstream of the fence in terms of those immediately upstream through a series of dimensionless correlations. Britter [5] takes a similar approach in deriving the algorithms to account for the effects of an isolated circular or square building. The predictions of the extended model of Cleaver *et al.* for instantaneous releases with the implemented algorithms of Britter were compared with some data from the Thorney Island field trials [30] and the BA propane field experiments [23, 36] and show a similar level of accuracy to a flat terrain model [10].

Webber *et al.* [57], deriving other obstacle algorithms, which they implemented to the conventional DRIFT (Dense Releases Involving Flammables and Toxics) model for instantaneous releases over flat and unobstructed terrain [54], followed the approach of Britter. They also started from the analysis of the experimental data of Britter [5] describing the behavior of steady heavy gas plumes as they interact with the fence. However, they do not fully agree with Britter's arguments. Webber *et al.* [57] argue that the evidence for a dependence on the Richardson number of the plume is slight and that the aspect ratio of the plume prior to the fence is a more important value. In the derivation of the Webber *et al.* [57] algorithms the following assumptions have been made:

- the contaminant flux of the steady plume is conserved;
- the plume advection velocity is not affected as it passes the fence;
- if the plume is sufficiently high before it reaches the fence it is unaffected by the fence;
- if it is initially lower than the fence then it mixes in the lee to a height controlled by the height of the fence;
- as it passes the fence its aspect ratio changes exactly as it would have done when undergoing the same dilution during advection in open terrain.

Britter [7] has stressed that no evidence has been presented to support this last hypothesis, and the authors make it at a first guess. He adds that the hypothesis is not unreasonable, there is no evidence to refute it, and if correct, it allows for a very simple and transparent inclusion in any dense gas dispersion code. Webber *et al.* [57] have proposed similar algorithms also for the effects of buildings. The experimental technique of Webber *et al.* [57] describes the influence of single, simple obstacles on the heavy plume and does not make allowance for the fence porosity nor for the density of the cloud. The results of the extended DRIFT model for instantaneous releases compare well with the WSL (Warren Spring Laboratory) repeat variability wind tunnel measurements [18] and the model predictions of minimal effect of the building are essentially consistent with the data from the Thorney Island field trial 26 [30]. It is important to note that both models described above do not attempt to account for flows in the neighborhood of an obstacle.

Steady state plume models are used for continuous grounded releases. They are developed in a similar manner as the box models. All the basic phenomena associated with the heavy gas behavior such as the horizontal spreading, exchange of the mass between the plume and the surrounding air, the plume heating are also described by ordinary differential equations. However, here the plume properties are averaged over plume slice in the crosswind and the equations are integrated with respect to the downwind distance. The plume cross section is assumed to be a rectangle. The rectangular or Gaussian profile is adjusted to this shape for concentrations.

As in the case of box models, it is generally not possible to extend the steady state plume models to complex and obstructed terrain. However, there are modifications of conventional steady state models for simple cases of non-flat and obstructed terrain. Modifications cover the following conditions:

- simple obstacles such as fences and buildings;
- inclined valleys.

The influence of simple obstacles downwind of the release on heavy gas plume is described in the work of Cleaver *et al.* [10]. Brighton [2], in turn, has described the model for releases into a building wake. Cleaver *et al.* [10] have introduced exactly the same obstacle algorithms to their conventional steady state plume model for a flat and unobstructed terrain as they introduced to their conventional box model. Tests of the extended model of Cleaver [10] for continuous releases show an excellent fit with the data from the Thorney Island field trials [30], Falcon series field trials [8] and BA propane field experiments [36] and have obtained a similar level of accuracy to the flat terrain model.

The model of Brighton [2] for heavy gas releases into a building wake is an extension of Vincent's simple wake model for passive releases [52, 53]. The model involves the use of flux conservation relations in the two-layer wake and some simple assumptions about the turbulent transfer process and mean flow structure. Some of the main assumptions and points worth noting are:

- the dimensions of the wake are based on correlations of Fracknell [16] which were derived from wind tunnel measurements,
- volume fluxes of gas and air are preserved on mixing (i.e. the gas and air are at the same temperature or have equal molar specific heats),
- the volume flux of air into the lower layer is taken to be zero,
- the volume fluxes between the two layers are taken to be identical.

It has limited application as it can be applied in situations in which the gas density affects the wake circulation and in addition the roof flow reattachment occurs. The model enables calculation of the concentrations in both the upper and lower layers but requires knowledge of various mixing coefficients. The two-layer model of Brighton [2] is introduced as one of two models into the WEDGE (Wake Effects on the Dispersion of Gases to the Environment) program [27].

As far as simple slopes are concerned, Britter has proposed a model for steady heavy gas plumes with friction and entrainment in an inclined valley [3]. No more information is available on this model.

Generalized steady state plume models can be considered an extension of the steady plume models in the sense that the spatial variation of concentrations and other parameters in the plume cross section does not need to follow Gaussian or rectangular profiles. Similarity profiles determined empirically are used to describe them. This allows us to model some of the physical processes more realistically. The concentration is expressed in terms of a centerline ground level concentration, vertical and horizontal dispersion parameters and width of the plume. These quantities are determined from a number of basic equations describing heavy gas mass conservation, air entrainment, horizontal crosswind gravity spreading and crosswind diffusion.

One example of the generalized steady state plume model extended to the obstructed terrain has been traced in the work of Webber *et al.* [57]. From a mathematical point of view the incorporation of Cleaver's *et al.* empirical algorithms for treatment of obstacles to the generalized plume models seems possible [10].

Webber *et al.* [57] have adapted the conventional DRIFT model for the continuous releases over flat and unobstructed terrain [55] to incorporate the nearest equivalent obstacle algorithms to the obstacle algorithms used in the DRIFT model for instantaneous releases. The difference lies in the assumption concerning contaminant mass conservation as here not the total mass of contaminant but the contaminant flux conserved as the cloud passes a fence. The extended DRIFT model for continuous releases has been tested using the data from some of the BA Hamburg field experiments showing an excellent agreement [23] and the wind tunnel BA TNO (nederlandse organisatie voor Toegepast Natuurwetenschappelijk Onderzoek: in Dutch, the Netherlands organization for applied research) experiments [13].

The one dimensional integral plume models are used to describe continuous, elevated releases (jets). They are based on the integration of conservation equations of the mass, mass of a dense gas, downwind and crosswind momentum and energy averaged over the jet cross section. The gravity, drag force of the ambient flow and momentum of the entrained air influence the plume path. The entrainment rate in these models is different from that for the models of grounded clouds. It mainly depends on the velocity shear between the elevated jet and the surrounding air. The cross section of the jet is assumed to be a circle, ellipse or rectangle. Similarity profiles are used to reintroduce spatial variability of plume variables over the plume cross section. No attempts to extend the conventional one dimensional integral plume models for the interaction of the jet with the simple obstacles have been traced. The analysis of data from the wind tunnel study on the building effects on heavy jet dispersion carried out by Schatzman *et al.* [45] seems a good starting point to attempt such extension.

The one or two dimensional shallow layer models are used for grounded releases. They are based on partial differential equations describing the principles of conservation of the mass, mass of a dense gas, momentum and energy averaged over cloud depth (two dimensional models) or over the cloud depth and the cloud width (one dimensional models). The entrainment of ambient air is usually modeled using the concept of the entrainment velocity. The pollutant cloud behavior is described using the variables changing in one or two dimensions in space and time. Shallow layer models are intermediate in complexity between the other integral models and the three dimensional fluid dynamics models.

As far as the influence of complex and obstructed terrain on heavy gas dispersion is concerned these models can deal with the inclined ground and thin vertical obstacles. Changing topography is included in these models quite easily by adding some terms to the momentum equation (the down slope buoyancy force). The influence of thin obstacles on the heavy gas dispersion is described by making use of the relation used in hydraulics

and proposed by Idelichik [24] for the flow through orifices with a sudden change in velocity and flow area. This approach has been invented by Wurtz [58]. It consists in adding extra terms to the momentum equations such as the enhanced drag and the enhanced entrainment. The enhanced drag is calculated using the relation of Idelichik [24]. The enhanced entrainment is calculated adding an extra term proportional to the wind velocity to the entrainment velocity in a region of one obstacle height upwind of an obstacle.

The inclined ground and unobstructed terrain can be handled by the following models: the two dimensional TWODEE (health and safety laboratory TWO DimEnsional shallow layer model for heavy gas dispersion) model [20, 21] and the two dimensional SLAM (Shallow Layer Model) model [40]. The predictions of the TWODEE model were compared with experimental data including some data from the BA Hamburg wind tunnel experiments (continuous and instantaneous releases in calm conditions over different slopes) [44]. Although no perfect agreement was reached, the model predictions are generally accurate (in terms of peak concentration comparison) to within a factor of three [20].

The treatment of inclined topography and simple thin obstacles is included in the following models: the one dimensional model of Wurtz [58] and two dimensional DIS-PLAY-2 (DISPersion using shallow LAYer modeling) model [51]. It is worth mentioning that in the DISPLAY-2 model the enhancement of entrainment is modeled not by increasing the entrainment but by adding locally an obstacle characteristic velocity. The model of Wurtz gives useful predictions in the presence of simple obstacles or on a sloped terrain. This is evident in Wurtz [58], based on the data from the BA propane field experiment EEC-57 (for the continuous release with a fence removed during the test) [23, 33, 34, 35] and some wind tunnel experiments by Britter [5] (for continuous releases with a two dimensional fence) and some BA Hamburg wind tunnel experiments (for instantaneous releases on a sloping floor [29]. The DISPLAY-2 model performance has been evaluated against theoretical results and the experimental data including the BA propane field experiments EEC-550/551 (for continuous releases with and without fence on flat ground) [23, 35], the BA Hamburg wind tunnel experiment DAT 638 (for instantaneous releases on inclined terrain) [29]. The model predictions are found to be in the reasonably good agreement with the theory and experiments [51].

It seems worth emphasizing that, in the simulations of heavy gas atmospheric dispersion carried out with the shallow layer models, it is possible to include the distortion of the wind field due to complex and obstructed terrain. The wind field can be obtained from a prognostic or diagnostic meteorological model prior to shallow layer model runs. This approach, however, requires large computational times and, therefore, is not used [20].

## Computational fluid dynamics models

This class of models is the most complex. The computational fluid dynamics models are three dimensional models, in which a full set of partial differential equations dependent on time and three spaces coordinates describing the principles of conservation of the mass, momentum, energy and dense gas mass, are solved. They generally provide the most detailed and complete description of heavy gas dispersion. These models are capable of modeling complex time dependent phenomena and take into account complex boundary conditions imposed by terrain and structures. These models are especially useful when the cloud interacts with arrays of obstacles such as buildings in urban areas or industrial areas, which also can have many pipe racks, tanks and other types of obstacles.

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The fundamental emphasis in computational fluid dynamics models is on the modeling the effects of turbulence. Turbulence is modeled using models of variable complexity. Currently the k-l turbulence model and the k-eps turbulence model are standard. In the k-l turbulence model one scalar transport equation for the turbulent kinetic energy (k) is solved. This is combined with an empirical relationship for the turbulence length scale (1) and the eddy viscosity hypothesis to calculate a distribution of effective turbulent viscosity. In the k-eps turbulence model one scalar transport equation for turbulent kinetic energy (k) and one for its rate of dissipation (eps) are used. These equations contain also a number of modeling constants whose values have been established by experiment. Eddy viscosity is calculated knowing the values of k and eps at each grid node. The new models of turbulence include the Reynolds stress models. They are based on transport equations for all components of the Reynolds stress tensor and the dissipation rate. The values of the Reynolds stress tensor components are obtained by solution of the differential equations of Reynolds stress components (differential models) or are calculated from a set of equations derived from the Reynolds stress equations (algebraic models). In the heavy gas dispersion over obstacles calculations the SSG (Speziale, Sarkar, Gatski) differential Reynolds Stress model [47] has been used. However the Reynolds stress models show superior predictive performance compared to eddy-viscosity models in cases, such as buoyant flows or free shear flows with strong anisotropy in this application the SSG model entailed increased CPU time without significant enhancement of accuracy of results [46].

Currently the ADREA-HF (Atmospheriki Diaspora Rypwn epi Edafous Anomalou: in Greek, the atmospheric dispersion of pollutants on irregular ground - Heavy Fluid) model [1] and the MERCURE-GL (a mythology name – Gas Lourds: in French, heavy gas) model [40] are the most often used models of the fluid dynamics models devoted especially to the heavy gas atmospheric dispersion. However, it is worth mentioning that recently the application of general purpose fluid dynamic codes increases [26, 42]. The treatment of obstacles in heavy gas atmospheric dispersion models may vary. In the MERCURY-GL model obstacles are defined by solid boundary points which approximate the shape of an obstacle. In the ADREA-HF model complex geometrical structures crossing the control volume/surfaces of a grid are treated using the notations of control volume porosity and area permeability. This approach is particularly attractive because an increase in topographic complexity or in obstacles does not increase the overall complexity. The necessary geometrical data are either given manually or generated automatically using the geometrical input processor DELTA-B. The MERCURE-GL model and the ADREA-HF model have been validated against a wide range of experimental data [7, 11] including the data for complex and obstructed terrain from the Thorney Island field trials (instantaneous release with a fence) [31], the BA propane field experiments (continuous release with an obstacle) [23, 34, 35], the BA Hamburg wind tunnel experiments (the continuous and instantaneous release with a steep slope) [44], the EMU ENFLO (Evaluation of Model Uncertainty, ENvironmental FLOw research centre) wind tunnel experiments (the continuous release in complex terrain with buildings) [19].

#### CONCLUSION

Since many heavy gas storage or production facilities are localized in non-flat terrain and surrounded by obstacles such as buildings, fences and installations of different geometries, the modeling of the heavy gas atmospheric dispersion over complex and obstructed terrain is worth special attention.

Future research in the area should include both experimental and modeling work. As it is known they complement each other. Experimental work helps to improve the basic understanding of the phenomena under study and provides data for the development and validation of the models. Modeling work allows the interpolation and the extrapolation of the information gained by laboratory and field experiments. Britter calls it the "repackaging" of the understanding of the phenomena [7]. It is worth stressing that the laboratory and field experiments are equally important and mutually beneficial. The field experiments are considered a "reality check" of the laboratory work and the laboratory studies are often used to plan the field studies.

In the context of this paper future modeling work is worth considering in more detail. It would be useful to suggest what approaches employed in heavy gas atmospheric dispersion models to describe the effects of complex and obstructed terrain on the behavior of heavy gases in the atmosphere are worth further attention, what specific tasks are to be carried out and what is to be done in relation to this subject in Poland. As far as the first issue is concerned it seems that all the approaches to describe the heavy gas atmospheric dispersion over complex and obstructed terrain are worth further attention even though there is always hesitation if the simple models have not been pushed too far. This opinion is supported by the fact that these approaches are used in different types of heavy gas dispersion models, which in turn differ in applications. Simpler methods are introduced to simpler heavy gas atmospheric dispersion models applied mainly in the routine calculations. The advanced techniques capable to describe the flow near complicated geometries are used in the sophisticated models applied mainly as research tools. This holds true even though the predictions from the models belonging to different classes when compared to the experimental data do not show equally encouraging results. It should be stressed that the results of the models validation can be compared only if the models belong to the same group and have been tested using the same procedure and the same experimental data [9, 11]. As far as some specific tasks are concerned it seems worth working on:

- improvement of some simpler approaches to estimate the effects of single obstacles such as fences or buildings on the behavior of the heavy gas clouds which can be introduced to the simpler integral models. For example, some of these approaches can be improved by making the allowance for such feature as the porosity of the obstacle. The next step is to focus on the description of the effects of the group of obstacles representative of an industrial site or urban environment [7, 14]. Since the flow and dispersion around a group of buildings is a complex and sensitive function of such parameters as spacing between the buildings, their dimensions, their arrangement to each other and to the wind direction, the approaches describing the effects of the group of obstacles should distinguish different flow regimes: the large separation, intermediate separation (the wake interference), skimming flow, small separation. The theoretical considerations related to this issue and a methodology consisting of flow charts which can be used to assist when undertaking dispersion calculations within building complexes have been already undertaken and provide a basis for the future work [22, 43];
  - incorporation of the information on the effects of complex terrain on the ambient flow to the shallow layer models. The wind field can be obtained from a prognostic

or diagnostic meteorological model prior to shallow layer model runs. The incorporation of this information into a shallow layer model should be relatively straightforward from a computational point of view [20];

further development of the turbulence modeling in the computational fluid dynamics models so the physics could be more realistically modeled. Additionally, the improvement in numerical techniques is very important as this can enable improving both dealing with the new turbulence modeling formulation and also it ensures that accurate and economical solutions are possible.

As far as the research in Poland in this area is concerned, it is worth stressing that not much work related to the development of the heavy gas dispersion modeling has been carried out. There is only one model of heavy gas atmospheric dispersion developed in our country up till now but it deals with flat and open terrain [17]. Taking into account the tasks to be done in the area of heavy gas dispersion modeling in the complex and obstructed terrain and the situation in Poland, it seems that Polish modelers should both undertake the work to improve the modeling methods and intensify actions to implement in Poland the models of different complexity developed and used abroad.

# REFERENCES

- [1] Bartzis J.G.: *ANDREA-HF: a three dimensional finite volume code for vapour cloud dispersion in complex terrain*, JRC lspra Report EUR 13580 EN, EC Joint Research Centre, lspra 1991.
- [2] Brighton P.W.M.: Heavy gas dispersion from sources inside buildings or in their wakes, [in:] Proceedings of the IchemE North Western Branch Symposium on Refinement of estimates of the consequences of heavy toxic vapour releases, UMIST, Manchester 1986.
- [3] Britter R.E., R.P. Cleaver, M.G. Cooper: Development of simple model for the dispersion of a denser then air vapour clouds over real terrain, MRSEG22 Report, British Gas plc, Research and Technology Midlands Research Station, Warf Lane, Solihill, West Midlands 1991.
- [4] Britter R.E., J. McQuaid: Workbook on the dispersion of dense gases, HSE contract research Report No 17/1988, Health and Safety Directorate, Sheffield 1988.
- [5] Britter R.E.: Experiments on some effects of obstacles on dense gas dispersion, SRD R407, UKAEA Safety and Reliability Directorate, Wigshaw Lane, Culcheth, Warrington 1989.
- [6] Britter R.E.: The atmospheric dispersion of dense gases, [in:] Proceedings of the Summer School, International Centre for Theoretical Physics, Trieste 1994.
- [7] Britter R.E.: Recent research on the dispersion of hazardous materials, University of Cambridge Report EC EUR 18198 EN, Directorate of Science, Brussels 1998.
- [8] Brown T.C., R.T. Cederwall, S.T. Chan, D.L. Ermak, R.P. Koopman, K.C. Lamson, J.W. McLure, L.K. Morris: *LNG Vapour barrier verification field trials*, Falcon series data Report, Final Report number 1990 GRI-89/0138, 1987.
- [9] Carissimo B., S.F. Jagger, N.C. Daish, A. Halford, S. Selma-Olsen, K. Riikonen, J.M. Perroux, J. Wurtz, J.G. Bartzis, N.J. Duijm, K. Ham, M. Schatzman, D.R. Hall: *The SMEDIS Database and validation exercise*, International Journal of Environment and Pollution, 16, 1–6 (2001).
- [10] Cleaver R.P., M.G. Cooper, A.R. Halford: Further development of a model for dense gas dispersion over real terrain, Journal of Hazardous Materials, 40, 85–108 (1994).
- [11] Daish N.C., R.E. Britter, P.F. Linden, S.F. Jagger, B. Carissimo: SMEDIS: Scientific model evaluation of dense gas dispersion model, International Journal of Environment and Pollution, 14, 39–51 (2000).
- [12] Directory of atmospheric transport and diffusion consequence assessment models, U.S. Department of Commerce, National Oceanic and Atmospheric Administration, FCM-13-1999, Washington DC 1999.
- Duijm N.J. (ed): Research on the dispersion of two-phase flashing releases, FLADIS-Final Report, TNO-ME-report R95, TNO, Apeldoorn 1995.
- [14] Duijm N.J.: Dispersion of dense gas and flashing releases, [in:] Materials from the Workshop on Modelling and mitigation the consequences of accidental releases of hazardous materials, New Orleans 1995.
- [15] Flacher A.: Experimentelle Untersuchung der Ausbreitung einer Schwergaswolke auf geneigtem Grund, Diplom Thesis, Institut f
  ür Fluiddynamik, ETH Z
  ürich, Z
  ürich 1994.

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[16]	Fracknell J.E.: <i>Parameters characterising dispersion in the near wake of buildings</i> , Journal of Wind Engineering and Industrial Aerodynamics, <b>16</b> , 97–118 (1984)
[17]	Galkowski A.: A unified model for pollutant dispersion in atmosphere and for consequence assessment, [in:] Models and techniques for health and environmental hazard assessment and management, M.J. Bo- rysiewicz (ed.), Institute of Atomic Energy, Otwock 2006.
[18]	Hall D.J., R.A. Waters, G.W. Marsland, S.L. Upton, M.A. Emmott: <i>Repeat variability in instantaneously releases heavy gas clouds – some wind tunnel model experiments</i> , Report LR 804 (PA), Warren Spring Laboratory, Gunnels Wood Road, Stevenage, Hertfordshire 1990.
[19]	Hall R.C. (ed.): Evaluation of model uncertainty (EMU) – CFD modelling of near-field atmospheric dispersion, Project EMU Final Report to the European Commission (Data CD also available with report), WS Atkins Doc No WSA/AM5017/R7, WS Atkins, Woocote Grove, Ashley Road, Epson, Surrey 1997.
[20]	Hankin R.K.S.: <i>Heavy gas dispersion over complex terrain</i> , PhD thesis, Trinity College, Cambridge University, Cambridge 1997.
[21]	Hankin R.K.S., R.E. Britter: TWODEE: the Health and Safety Laboratory's shallow layer model for heavy gas dispersion. Part I: Mathematical basis and physical assumptions, Part II: Model validation, Journal of Hazardous Materials, <b>66</b> , 211–237 (1999).
[22]	Hanna S.R., R.E. Britter, P. Franzese: The effects of roughness obstacles on the flow and dispersion at industrial and urban sites, AICHE/CCPS, 3 Park Avenue, New York 2002.
[23]	Heinrich M., R. Scherwinsky: <i>Research on propane releases under realistic conditions-determination of gas concentrations considering obstacles</i> , TUV Final Project Report 123UI00780, TUV Norddeutchland, 1990.
[24] [25]	Idelchik I.E.: <i>Handbook of Hydraulic Resistance</i> , Hemisphere, Washington 1986. Kukkonen J., J. Nikimo: <i>Modelling heavy gas cloud transport in sloping terrain</i> , Journal of Hazardous Materials, <b>31</b> , 155–176 (1992).
[26]	Luketa-Hanlin A., R.P. Koopman, D.L. Ermak: On the application of computational fluid dynamics codes for liquefied natural gas dispersion, Journal of Hazardous Materials, <b>140</b> , 504–517 (2007).
[27] [28]	Luong H.Y.: WEDGE validation report, WS Atkins Internal Report No. AM5109-R2, 1997. Markiewicz M.: Modelling of heavy gas dispersion in Poland, [in:] Environmental Engineering, L. Pawłowski M Dudzińska A Pawłowski (eds) Taylor and Francis London 2007 pp. 341–348.
[29]	Marotzke K.: Wind tunnel modelling of density current interaction on an inclined plan, [in:] Proceedings of the CEC project BA meeting, Meteorological Institute of Hamburg University, Lathen 1989.
[30]	EUR 10029 EN, Brussels 1985.
[31]	McQuaid J.: Heavy gas dispersion trials at Thorney Island, Journal of Hazardous Materials, II, 21 (1985).
[32]	Mercer A., C. Bartholome, B. Carissimo, N. Duijun, H. Giesbrecht: <i>Heavy gas dispersion expert group</i> <i>final report</i> , CEC Model Evaluation Group, Brussels 1996
[33]	Nielsen M., N.O. Jensen: <i>Research on continuous and instantaneous gas clouds</i> , Journal of Hazardous Materials, <b>21</b> , 101–104 (1989).
[34]	Nielsen M.: Preliminary treatment of meteorological data from project BA dense gas experiments, Report Riso-M-2882, Riso National Laboratory, Roskilde 1990.
[35]	Nielsen M., N.O. Jensen : <i>Continuous releases. dense gas experiments with obstacles</i> , Final report on Project BA.X2 Riso-M-2923, Riso National Laboratory, Roskilde 1991.
[36]	Nielsen M., M. Heinrich, R. Scherwinsky: <i>Research on continuous and instantaneous gas clouds Part II</i> , Journal of Hazardous Materials, 26, 219–244 (1991)
[37]	Nielsen M.: Dense gas dispersion in the atmosphere, PhD, Riso National Laboratory, Roskilde 1993.
[38]	Nielsen M.: Comment on: A model of the motion of a heavy gas cloud released on a uniform slope, Journal of Hazardous Materials, <b>48</b> , 251–258 (1996).
[39]	Ott S., M. Nielsen: <i>Shallow layer modelling of dense gas clouds</i> , Riso-R-901 EN, Riso National Laboratory, Roskilde 1996.
[40]	Riou Y.: Comparison between MERCURE GL: code calculations, wind tunnel measurements and Thor- ney Island field Trials, Journal of Hazardous Materials, 16, 247–265 (1987).
[41]	Ross A.N., P.F. Linden, S.B. Danziel: A study of three-dimensional gravity currents on uniform slope, Journal of Fluid Mechanics, <b>453</b> , 239–261 (2002).
[42]	Scargiali F., E. Di Rienz, M. Ciofalo, F. Grisafi, A. Brucato: <i>Heavy gas dispersion modelling over topo-graphically complex mesoscale: a CFD approach</i> , Process Safety Environmental Protection, <b>83 (B3)</b> , 242–256 (2005).
[43]	Scaperdas A., C.R. Hebden: Source term modelling of releases within building complexes, Research re-

port 064, WS Atkins Consultants Ltd, Woodcote Grove, Ashley Road, Epsom 2003.

- [44] Schatzmann M., K. Marotzke, J. Donat: Research on continuous and instantaneous heavy gas clouds, EV report 91-026/r.24/HVG, University of Hamburg, Hamburg 1990.
- [45] Schatzmann M., W.H. Snayder, R.E. Lawson Jr.: Building effects on heavy gas jet dispersion, [in:] Proceedings of International Conference and Workshop on Modelling and mitigating the consequences of accidental releases of hazardous materials, New Orleans 1995, pp. 359–378.
- [46] Sklavounos S., F. Rigas: Validation of turbulence models in heavy gas dispersion over obstacles, Journal of Hazardous Materials, A108, 9–20 (2004).
- [47] Speziale C.G., S. Sarkar, B. Gatski: Modelling the pressure strain correlation of turbulence: an invariant dynamical systems approach, Journal of Fluid Mechanics, 227, 245–272 (1991).
- [48] Tickle G.A.: A model of the motion and dilution of a heavy gas cloud released on a uniform slope in calm conditions, Journal of Hazardous Materials, 49, 29–47 (1996).
- [49] User's guide to TSCREEEN. A model for screening toxic air pollutant concentrations, EPA-450/B-94-023, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1994.
- [50] VDI Guidelines 3783 Part II Environmental Meteorology. Dispersion of heavy gases, 1990.
- [51] Venetsanos A.G., J.G. Bartzis, J. Wurtz, D.D. Papailiou: DISPLAY-2: a two-dimensional shallow layer model for dense gas dispersion including complex features, Journal of Hazardous Materials, A99, 111– 144 (2003).
- [52] Vincent J.H.: Model experiments on the nature of air pollution transport near buildings, Atmospheric Environment, 11, 765–774 (1977).
- [53] Vincent J.H.: Scalar transport in the near aerodynamic wakes of surface mounted cubes, Atmospheric Environment, 12, 1319–1322 (1987).
- [54] Webber D.M., S.J. Jones, G.A. Tickle, T. Wren: A model of the dispersion dense gas cloud and the computer implementation DRIFT: Part I Near-instantaneous releases, HSE/SRD R586, Wigshaw Lane, Culcheth, Cheshire 1991.
- [55] Webber D.M., S.J. Jones, G.A. Tickle, T. Wren: A model of dispersion dense gas cloud and the computer implementation DRIFT. Part II Steady continuous releases, HSE/SRD R587, Wigshaw Lane, Culcheth, Cheshire 1991.
- [56] Webber D.M., S.J. Jones, D. Martin: A model of the motion of a heavy gas cloud released on a uniform slope, Journal of Hazardous Materials, 33, 101–122 (1993).
- [57] Webber D.M, S.J. Jones, D. Martin: Modelling the effects of obstacles on the dispersion of hazardous materials, [in:] Proceedings of International Conference and Workshop on Modelling and mitigation the consequences of accidental releases of hazardous material, New Orleans 1995, pp. 379–403.
- [58] Wurtz J.: A transient one dimensional shallow layer model for dispersion of denser than air gases in obstructed terrain under non-isothermal conditions, Report EUR 15343 EN, Joint Research Centre, Ispra 1993.

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#### MATEMATYCZNE MODELOWANIE ROZPRZESTRZENIANIA SIĘ W ATMOSFERZE GAZÓW CIĘŻSZYCH OD POWIETRZA W TERENIE O SKOMPLIKOWANEJ TOPOGRAFII, W POBLIŻU BUDYNKÓW I PRZESZKÓD TERENOWYCH

W artykule przedstawiono możliwości uwzględnienia w modelach rozprzestrzeniania się w atmosferze gazów cięższych od powietrza opisu wpływu topografii, budynków i przeszkód terenowych na rozprzestrzenianie się gazów cięższych od powietrza. Modele podzielono na trzy grupy i wyróżniono: modele fenomenologiczne (empiryczne), modele pośrednie (inżynierskie) i modele obliczeniowej dynamiki płynów (badawcze). Każdą grupę modeli scharakteryzowano oddzielnie. Zasadnicze cechy modeli przedstawiono skrótowo. Przytoczone przykłady modeli rozprzestrzeniania się w atmosferze gazów cięższych od powietrza, uwzględniające wpływ topografii, budynków i przeszkód terenowych na przemieszczanie się gazów cięższych od powietrza, są rezultatem prac prowadzonych w krajach Unii Europejskiej i Stanach Zjednoczonych. W Polsce jak dotąd nie opracowano takiego modelu. W artykule zwrócono uwagę na konieczność prowadzenia dalszych prac nad wpływem topografii, budynków i przeszkód na rozprzestrzeniane się gazów cięższych od powietrza w atmosferze. Przyszłe badania winny uwzględniać zarówno prace pomiarowe jak i matematyczne modelowanie. W kontekście tej publikacji warto bardziej dokładnie rozważyć prace nad modelami. Wydaje się, że wszystkie podejścia stosowane przy opisie rozprzestrzeniania się gazów cięższych od powietrza w terenie o skomplikowanej topografii, w pobliżu budynków i przeszkód terenowych warte są dalszej uwagi. Opinię tę popiera fakt,

że różne podejścia są stosowane w różnych rodzajach modeli gazów cięższych od powietrza, które z kolei mają różne zastosowania. Prostsze metody są wprowadzane do prostszych modeli gazów cięższych od powietrza stosowanych głównie w rutynowych obliczeniach. Zaawansowane techniki zdolne do opisu przepływu w pobliżu skomplikowanych geometrycznie obiektów są używane w wyrafinowanych modelach stosowanych głównie jako narzędzia badawcze.