**Studies in Systems, Decision and Control 552**

Vitalii Babak Artur Zaporozhets Editors

# Systems, Decision and Control in Energy VI

Volume II: Power Engineering and Environmental Safety



# **Studies in Systems, Decision and Control**

Volume 552

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# Systems, Decision and Control in Energy VI

Volume II: Power Engineering and Environmental Safety



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ISSN 2198-4182 ISSN 2198-4190 (electronic) Studies in Systems, Decision and Control<br>ISBN 978-3-031-67090-9 ISBN ISBN 978-3-031-67091-6 (eBook) <https://doi.org/10.1007/978-3-031-67091-6>

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### **Preface**

This book stands as a compendium poised at the crossroads of human progress and environmental equilibrium, encapsulating the intricate interplay between burgeoning energy demands and the imperatives of ecological sustainability. In the annals of global energy evolution, the year 2023 emerges as an epochal threshold, marked by a confluence of transformative dynamics reshaping the contours of power engineering and environmental stewardship.

At its core, this scholarly exposition endeavors to dissect and illuminate the nuanced facets of the energy landscape, offering a comprehensive elucidation of the defining features that delineate the trajectory of energy development in this pivotal year. It serves as an indelible testament to the relentless pursuit of sustainable energy solutions amidst a backdrop of intensifying environmental concerns and burgeoning global energy needs.

The defining hallmark of 2023's energy panorama lies in the resounding impetus towards sustainability—a seismic paradigm shift echoing across industries, policies, and societal aspirations. Heightened awareness of climate change, environmental degradation, and the imperatives of decarbonization propel an unprecedented surge towards renewable energy alternatives. Solar, wind, hydro, geothermal, and other sustainable modalities witness not only technological advancements but a transformative surge in accessibility, affordability, and scalability, redefining the global energy matrix.

Within this transformative landscape, innovation emerges as the fulcrum catalyzing the metamorphosis of energy systems. Breakthroughs in energy storage technologies, smart grid optimization, and decentralized energy solutions orchestrate a symphony of efficiency, enabling the seamless integration of intermittent renewable sources while ensuring grid stability and resilience. The amalgamation of artificial intelligence, big data analytics, and energy systems heralds a new frontier of smart, adaptive energy networks, revolutionizing the paradigm of energy consumption and management.

Furthermore, the geopolitical milieu assumes heightened significance in shaping the contours of global energy dynamics. Interwoven with alliances, trade dynamics, and international agreements, geopolitics exerts profound influences on energy security, infrastructural investments, and the trajectory of sustainable energy transitions. Collaborative endeavors and multilateral initiatives reverberate as essential instruments in navigating the complexities of a globally interconnected energy landscape.

However, amid the triumphant strides towards a sustainable energy future, challenges persist. The intricacies of phasing out legacy infrastructures, addressing socioeconomic disparities, navigating policy ambiguities, and fostering inclusive energy transitions underscore the labyrinthine complexities that necessitate astute navigation and multifaceted solutions.

This book aspires to be a scholarly compass guiding academia, policymakers, industry practitioners, and stakeholders through the labyrinth of contemporary energy dynamics. Through meticulous analyses, empirical insights, and visionary perspectives, this compendium endeavors to illuminate the path towards a harmonious coexistence of burgeoning energy exigencies and the imperatives of environmental preservation, forging a trajectory that sustains both progress and planetary well-being.

Kyiv, Ukraine December 2023

Vitalii Babak Artur Zaporozhets

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**Electric Power Engineering**

## <span id="page-12-0"></span>**Mathematical Means to Assess Consequences of Chemical Accidents with Heavy Gas Emissions**



#### **Andrii Iatsyshyn [,](http://orcid.org/0000-0001-5508-7017) Teodoziia Yatsyshyn, Kyrylo Nikolaiev, IhorNeklonskyi<sup>n</sup>, Andrii Melnychenko<sup>n</sup>, and Volodymyr Artemchuk <b>D**

**Abstract** This article presents mathematical models classification of heavy gas dispersion according to various criteria. Empirical, engineering and computational hydrodynamic (research) models are described in detail, and their advantages and disadvantages are shown. Engineering models are also analyzed. It includes box models for instantaneous emissions, uniform or Gaussian plume models, generalized plume models, integral-jet models, and shallow-layer models. Examples of research models are given and their practical implementation is demonstrated.

**Keywords** Atmospheric air pollution · Heavy gas · Mathematical models · Modeling

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<sup>©</sup> The Author(s), under exclusive license to Springer Nature Switzerland AG 2024 V. Babak and A. Zaporozhets (eds.), *Systems, Decision and Control in Energy VI*, Studies in Systems, Decision and Control 552, [https://doi.org/10.1007/978-3-031-67091-6\\_23](https://doi.org/10.1007/978-3-031-67091-6_23)

#### **1 Introduction**

Assessment of environmental risk associated with the production, storage, and transportation of flammable and toxic gases involves quantifying dispersion occurring in accidental release cases. The spread of dangerous chemicals occurred during such emissions. It threatens the life and health of enterprise service personnel and the population in the surrounding area. Environmental pollution is observed during such accidents. Severe destruction is possible in large areas as a result of chemical explosions. There is a danger to all living creatures within the contaminated area  $[1-6]$  $[1-6]$ .

Efficient solutions for emergency, rescue, and other urgent works in the emergency zones require systematic, mathematical, and software for rapidly adopting appropriate management decisions at all stages of such situations development [\[7](#page-25-2)[–12](#page-26-0)]. Therefore, we will describe in detail various models regarding heavy gas dispersion, the principles of their construction, and their features.

#### **2 Research Results**

Released into the atmosphere substances with bigger than atmospheric air are called heavy or dense gases. Heavy gas dispersion differs from the dispersion of neutral or positively buoyant gases. Special models were developed to describe this process [\[13](#page-26-1)– [16\]](#page-26-2). However, mathematical models of heavy gas dispersion differ in their description and complexity.

Mathematical models of heavy gas dispersion can be classified according to various criteria. Most often, the criteria are the following: mathematical principles, type of emission source, and the complexity of the model. Dispersion models of heavy gas are divided into three groups according to the last criterion. These models are known as phenomenological (empirical), intermediate (engineering), and computational hydrodynamic (research) models. Engineering models include box models for instantaneous emissions, uniform or Gaussian plume models, generalized, integral-jet models, and shallow-layer models. Let's consider these models in detail.

#### **3 Empirical Models**

The description of heavy gas cloud dispersion in the empirical models is based on a series of nomograms or simple correlations. They are built using measurements results of many field and laboratory experiments [\[14](#page-26-3), [17\]](#page-26-4). These experiments studied ground-level emissions from instantaneous and continuous sources. They are related to grassy plain terrain and the neutral stability of the atmosphere. The measured concentrations were averaged over a period lasting from 3 to 10 min. The influence of

the atmosphere stability state, surface roughness, and averaging time was neglected to obtain the main dependences. Therefore, available data did not show a strong influence of these parameters on the gas dispersion density. Concentration in the center of the heavy gas cloud is calculated based on different ratios for instantaneous and continuous emissions in the gravity constant, the density difference between the gas and surrounding air, emission volume or velocity of the emission flow, and external wind speed.

In the model of Britter and McQuaid  $[18]$  $[18]$ , the concentration at ground level  $(C_m)$ along the central line is estimated with the initial concentration  $(C<sub>o</sub>)$  as a function of two dimensionless variables: dimensionless distance and the original Richardson number. Equations of continuous and instantaneous emissions have the following form.

$$
\frac{C_m}{C_o} = f_c \left( \frac{x}{(V_{co}/u_h)^{1/2}}, \frac{g(\rho_{co} - \rho_a)V_{co}^{1/2}}{\rho_a u_h^{5/2}} \right),
$$
\n
$$
\frac{C_m}{C_o} = f_i \left( \frac{x}{(V_{io})^{1/3}}, \frac{g(\rho_{co} - \rho_a)V_{io}^{1/3}}{\rho_a u_h^2} \right),
$$
\n(1)

where

*x*—distance downwind from the source; *Vco*—emission rate; *uh*—wind velocity at the height *h*;  $\rho_{co}$ —initial density of the emitted gas; ρ*a*—ar density;

*g*—gravitational constant;

*Vio*—discharge volume.

#### **4 Engineering Models**

Engineering models can be divided into five groups: box models for instantaneous emissions, uniform or Gaussian plume models, generalized plume models, integraljet models, and shallow-layer models. The last one is the most complex model among engineering models. They differ from other models of this group by the ability to consider the effects of topography and dimensionality.

#### *4.1 Box Models for Instantaneous Emissions*

Box models for instantaneous emissions describe jets (flows) of heavy gases. In these models, it is assumed that the pollution jet forms a homogeneous cylinder (Fig. [1](#page-15-0)),



where *H*, *R*—jet height and radius,  $u_c$ —jet transfer velocity,  $u_a$ —wind velocity,  $u_t$ ,  $u_e$ —upper and limit speed of air intake,  $u_f$ —gravitational frontal velocity [[18\]](#page-26-5).

The main variables of the jet (its radius, mass, and enthalpy) are obtained by numerical integration of the basic ordinary differential equations to time. Basic equations represent the horizontal spread of the layer, conservation of mass and energy.

Other jet variables are calculated from additional equations. Horizontal propagation affecting the cloud radius is estimated using the gravity front velocity.

The mass exchange between the jet and atmospheric air occurs through the top and edge of the cylinder. The inlet velocities describe it. Values of these parameters depend on the intensity of turbulence, the difference in the density of the emission and environment, and the transport speed of the leak. An increase in the temperature of the emission due to its contact with the ground and air is introduced in a straight line. The jet spreads in still air or moves with the wind. The transport velocity of the jet is calculated based on the captured momentum or wind speed. Concentration averaged over the box's volume is calculated as the ratio of the released substance mass to the box volume.

The main equations in the box model include equations of the horizontal spread of the layer:

$$
\frac{dR}{dt} = u_f,\tag{2}
$$

Equation of involved masses:

$$
\frac{dM_a}{dt} = \rho_a(\pi R^2)u_t + \rho_a(2\pi RH)u_e,\tag{3}
$$

<span id="page-15-0"></span>



Energy equation:

$$
M\frac{dh_c}{dt} = \frac{dM_a}{dt}(h_a - h_c) + E_f(\pi R^2),\tag{4}
$$

where:

*R, H, M, h<sub>c</sub>*—radius, height, mass and enthalpy per unit mass;

 $\rho_a$ , *Ma, h<sub>a</sub>*—atmospheric air jet density, involved mass and enthalpy per unit mass;

 $u_f$ —gravitational frontal velocity;

 $u_e$ ,  $u_t$ —capture velocities for the edge and top of the jet;

 $E_f$ —heat flow transmitted by the jet per unit area of the underlying surface.

The equations form a set of three coupled linear differential equations that can be solved numerically for the independent variables  $R$ ,  $M_a$ , and  $h$ . Gravitational velocity  $u_f$  is usually calculated by the gravity formula

$$
u_f = c_1 \left(\frac{g(\rho_c - \rho_a)H}{\rho_a}\right)^{1/2},\tag{5}
$$

where  $\rho_c$ —jet density.

Edge involving velocity  $u_e$  is usually scaled by  $u_f$  and defined as:

$$
u_e = c_2 u_f, \tag{6}
$$

where  $c_2$ —constant,  $0.6 < c_2 < 0.9$ .

Correlations of the following form are usually used for the upper involving rate.

$$
u_{t} = u_{*} \left( \frac{k}{1 + c_{3} \frac{g(\rho_{p} - \rho_{a})H}{\rho_{a} u_{*}^{2}}}\right),
$$
\n(7)

where;

 $\kappa$ —the Karman constant, which is equal to 0.4;

 $c_3$ —is a constant whose value can be deduced from laboratory experiments. For example, Britter suggests a value of 0.125.

It is enough to fulfill one of the following criteria to determine the moment of transition to passive dispersion: density difference is less than the specified value, or growth of the cloud radius is less than the specific value.

The jet position center is the equation.

$$
\frac{dx}{xt} = u_c,\tag{8}
$$

where  $u_c$ —transport speed of the jet.

Box models are built on this simple approach. They satisfactorily reproduce many aspects of field and laboratory experiments. Examples of box models include the GASTAR model, the HEGABOX model in the HGSYSTEM computer package, the IIT Heavy Gas Model I, the DENZ-EDF model, and many others.

In general, most box models assume a flat, uniform terrain. Only some models describe scattering on slopes or through fences and obstacles. Some of the models in this group are adapted to continuous terrestrial emissions of heavy gases. A series of rectangular jets then simulate the plume.

#### *4.2 Uniform or Gaussian Plume Models*

Uniform or Gaussian plume models are used for continuous steady-state emissions of heavy gases. They are designed in the same way as box models for instantaneous emissions. All the main phenomena related to the release of upwelling gases are described by ordinary differential equations similar to those in box models. These phenomena include horizontal propagation, mass transfer between the plume and the surrounding air, and heating. However, these equations are integrated concerning the downwind distance. The main variables are the average mass flow through the plume cross-section, the enthalpy flow, and the width of the plume. The plume moves downwind along with the wind speed. The cross-section of the plume is assumed to be rectangular (Fig. [2](#page-17-0)), where *E*—emission rate from the source, *H, b*—height, and width of the plume cross-section, respectively,  $u_c$ ,  $u_a$ —plume and wind speed,  $u_f$  horizontal velocity of propagation,  $u_t$ ,  $u_e$ —upper and edge capture of air velocities [[18\]](#page-26-5).



<span id="page-17-0"></span>**Fig. 2** Scheme of the plume model for heavy gas emissions [[18](#page-26-5)]



<span id="page-18-0"></span>**Fig.3** Scheme of the generalized plume model for heavy gas emissions [[18](#page-26-5)]

#### *4.3 Generalized Plume Models*

The HAGADAS model from the HGSYSTEM computer package and the DEGADIS model are examples of generalized plume models. Gas emission occurs from a rectangular source at ground level. The plume comprises horizontally uniform cross sections with Gaussian edges in the horizontal direction and an exponential profile in the vertical direction in both models. The mean transport rate in the plume is determined using a power-law profile for the wind speed. The geometry of the crosssection of the torch with similarity profiles choosing the drop in concentration and its effective characteristics are shown in Fig. [3](#page-18-0), where *E* emission rate from the source,  $H_{\text{eff}}$ ,  $B_{\text{eff}}$ —effective height and effective plume half-width,  $u_{\text{eff}}$ ,  $u_a$ —practical plume and wind speed,  $u_f$ —horizontal velocity of propagation,  $u_t$ ,  $u_e$ —upper and edge capture of air velocities, *b*—half-width of the crosswind along which the concentration at ground level is equal  $c_A$ ,  $S_y$ —dispersion coefficient of the crosswind which determines Gaussian decline of the concentration at a greater distance of the crosswind,  $S_z$ —vertical dispersion coefficient determining the steep attenuation [\[18](#page-26-5)].

#### *4.4 Integral-Jet Models*

Integral jet models describe continuous, intense, or powerful emissions of heavy gases. They are based on integrating equations of conservation of mass, species, downwind and crosswind momentum, and energy averaged over the jet cross-section. These equations directly predict jet variables such as concentration, jet velocity, radius, and enthalpy. In steady-state integral models, the jet variables are evaluated

<span id="page-19-0"></span>

as a function of downwind distance. These variables are estimated as a function of downwind distance and time in more general time-dependent models. The crosssection of the jet is considered a circle, an ellipse, or a rectangle. Uniform, Gaussian, or similarity profile describes the spatial variability of the jet variables in the crosssection.

A set of fundamental equations in the integral models for stationary jet emissions assumes that the axial line of the jet remains in the force of gravity of the wind and takes the form (Fig. [4](#page-19-0)), where *S*—linear coordinate of the jet axis curve,  $\Theta$  is the angle between the axial line of the jet and the horizontal axis,  $R$ —jet radius,  $u_c$ ,  $u_a$ —jet and wind speed,  $u_e$ —air intake speed [[18\]](#page-26-5).

Examples of stationary integral plume models include the HMP model, the Ooms model, the Khan and Abbasi model, AEROPLUME and HFPLUME models in the SYSTEM package. CLOUD model can follow steady state or transient conditions.

#### *4.5 Shallow-Layer Models*

One or two-dimensional shallow-layer models are used for terrestrial emissions. They are based on partial differential equations describing the conservation principles of mass, species, momentum, and energy averaged over cloud depth. This type of averaging is convenient due to the cloud geometry. Its vertical size is small compared to its horizontal size. The behavior of pollutant clouds is described by variables varying in one or two dimensions in space and time. The top of the cloud is rugged to determine in reality, and vertical concentration distribution is used to select it. The removal rate describes a mass exchange between the cloud and the atmospheric air. Complex topography is quickly introduced by adding some terms to the momentum equations. This is an advantage compared to simpler models. They are generally not suitable for complex topography.

SLAB model and DISPLAY 1 model are examples of one-dimensional shallow layer models. TWODEE model and DISPLAY 2 model are examples of twodimensional external layer models.

#### **5 Exploratory Models**

Exploratory models are three-dimensional models where a complete set of partial differential equations dependent on time and three spatial coordinates is solved. It describes the conservation principles of mass, momentum, energy, and matter [\[19](#page-26-6)]. These models can be applied to any emission scenario, terrain, or meteorological conditions. A description of the physical processes of the dispersion of heavy gases is detailed and complete. Some of these models include the concentration fluctuation model [\[20](#page-26-7)].

Models FEM3, MARIAH, MDPG, HEAVYGAS, MERCURE-GL, ANDREA are examples of exploratory models.

*Dense Gas Dispersion Model (DEGADIS)* [[21](#page-26-8)]—is a mathematical dispersion model that can be used to simulate the transport of toxic chemical emissions into the atmosphere. The range of its applications includes:

- continuous, instantaneous, finite duration, and time-varying emissions;
- emissions with negative buoyancy and neutral buoyancy;
- emissions at ground level with low momentum;
- emissions of gases or aerosols at ground level or elevation, directed upwards.

The model simulates only one set of meteorological conditions and, therefore, should not be applied for periods exceeding 1 or 2 h. The simulation is performed on a flat area without obstacles. Surface roughness characteristic for such an area does not make up a significant proportion of the depth of the dispersion layer. The model does not characterize the density of aerosol-type emissions; the user should estimate it himself before the simulation. DEGADIS can be used as an advanced modeling approach to estimate short-term environmental concentrations (averaging time of 1 h or less) and expected area of exposure for concentrations above specified threshold values for toxic chemical releases. This is particularly useful when density effects are suspected to be essential and when screening estimates of ambient concentrations exceed levels of concern.

The model simulates only one set of meteorological conditions and receives no real-time meteorological data. Contaminant data must be entered interactively or from a file for each run, as there is no chemical database. The terrain is assumed to be flat and without obstacles. Required inputs include emission rate, area of emission and duration of emission, chemical characteristics, stack parameters, and standard meteorological data. The receptor input consists of the desired averaging time, aboveground height of receptors, and maximum distance between receptors. Figure [5](#page-21-0) shows a validation study of the DEGADIS 2.1 model in field studies and a wind tunnel.



<span id="page-21-0"></span>**Fig. 5** Unobstructed Predicted and Measured Concentration (LNG Field Trials: Maplin Sands 27, 34, 35; Burro 3, 7, 8, 9; Coyote 3, 5, 6; Other Field Trials: Thorney Island 45, 47; Wind Tunnel Experiments: CHRC A; BA-Hamburg DA0120 (Unobstructed), DAT223 (Unobstructed 2); and BA-TNO TUV01, FLS.) [[22](#page-26-9)]

The model automatically writes an output file without a graphic image. The file consists of the following data: input data; plume centerline height, mole fraction, concentration, density, and temperature at each downwind distance; sigma y and sigma z values at each specified downwind distance; centerline distance for two specified concentrations at a user-specified receptor height, etc.

*Air-Force Dispersion Assessment Model (ADAM)* [[23\]](#page-26-10) is a PC-based dispersion model. It allows the user to specify output parameters immediately after the emission or to select output data from the parameters menu. However, the output data must correspond to either an instantaneous release or a steady-state continuous release; the model cannot work with a burst of limited duration. Also, ADAM is not designed for powerful emissions. ADAM contains an algorithm for dealing with scattering from jets; it considers the jet as being on the ground and horizontally aligned with the wind.

ADAM has a chemical database where the user should select input chemicals to run the model. The database contains eight chemicals and can be expanded. Other user-supplied inputs are the concentration contour and the averaging time.

The output of ADAM is a visualization of the gas cloud at a given concentration level and a table showing the amount of time passed by the cloud, its speed, and the width of the contour. ADAM also displays peak concentrations as a function of distance, and the peak dose can be calculated as a function of distance for the specified averaging time if the pollutant release is instantaneous. In both cases, the information is calculated for the center line of the contour. ADAM cannot determine the time history of concentration at specific points.

*HGSYSTEM* [\[24](#page-27-0)]—is a PC-based system consisting of seven different models, namely: (1) HF (hydrogen fluoride) spill from a vessel (HFSPILL); (2) spread/ evaporation from the liquid pool (EVAP); (3) it calculates the properties of anhydrous hydrogen fluoride (HF) after a flash (temperature, liquid fraction) (HFFLASH); (4) jet flow, HF near-field dispersion (HFPLUME); (5) jet flow, near-field dispersion of an ideal gas (PLUME); (6) dispersion of heavy gas at ground level (HEGADIS); (7) increased passive dispersion (PGPLUME). In some cases, the models can be used together and sequentially. That is, the output data of one model can be used as input data for another model. Modeling capabilities can be complex since multiple models may be involved in each scenario [[25\]](#page-27-1).

HGSYSTEM contains scripts that guide users through the process. The model that includes pool evaporation (model 2) requires the most considerable input of liquid release properties. HF modeling (models 3 and 4) requires less input because the chemical information already exists in the model itself. Scattering in the near field (model 5) modeling jet flow involves a description of the emission and environmental conditions. Finally, the enhanced passive dispersion simulation (number 7) requires input from the near-field model and selected environmental and dispersion data.

Each of the seven models requires detailed data on the thermal properties of the gas, its initial concentration, area, a complete description of environmental conditions, and terrain characteristics. HEGADIS is a heavy gas dispersion model in the atmosphere. It should be implemented after the source model is defined.

PGPLUME generates tabular data for the downwind distances from the source for the output data. Molar concentration is reported in the plume vertical crosssection typical to the transport direction. It is a steady-state or limited-duration release model, so there are no time histories. HEGADIS uses two post-processing algorithms to calculate the result. The HSPOST algorithm (used for steady-state emissions) determines the concentration at any point *(x, y, z)*. It also reports concentrations, geometries, and temperatures for points along the ground in line with the plume axis. This post-processor can also calculate tabular or graphical results for limited-duration releases. HTPOST (used for interim releases) averages the time series concentrations reported from the temporary version of HEGADIS. This post-processor can output data at a specific time, or the user can specify a point and obtain a time series of concentration.

**SLAB model** was developed by the authors of the American Meteorological Society (AMS) [\[26](#page-27-2)]. It is a model of the surface or lower mixed layer where all quantities (scalar and vector) are homogenized entirely and instantaneously. This is a PCbased model of dispersion of denser-than-air emissions. The assumption is that the

processes affecting the mixed layer as a whole act slowly compared to the mixing time of the large eddies that stir the layer. This approximation treats the atmospheric boundary layer if variables such as potential temperature, momentum, pollutants, and humidity are uniform with height.

Idealization for the atmospheric boundary layer assumes uniform (well-mixed) values with height within the boundary layer bounded by discontinuity (or jump) at the top of the boundary layer. Another name for this approach is the SLAB model. The homogeneous part of the boundary layer behaves similarly to a uniform slab of material. Such jump or step models are reasonable simplifications for the convective boundary layer, where energetic thermals keep the boundary layer well mixed. However, they are poor idealizations for statically stable and neutral boundary layers.

Figure [6](#page-23-0) shows the JR II 2015 wind speed profile (Jack Rabbit data) and corresponding simulated SLAB and SLAB-M values from 2 to 2000 m.

This model type is popular due to its simplicity, requiring only predictions of mean variables in the mixed layer and changes in varied layer depth. The actual boundary layer is often sufficiently well mixed that the uniform SLAB approximation is quite good on sunny days over land.

SLAB can be applied to four types of emissions: ground-level evaporation basin, raised horizontal jet, plume or introduced vertical jet, and instantaneous volume source [[23\]](#page-26-10). All sources except the evaporation basin. It can be characterized as aerosols. The model can simulate several sets of meteorological conditions in a single run. It does not accept any real-time meteorological data. Data is entered directly into the model from an external file. Inputs include source type, source properties, spill properties, field properties, and standard meteorological parameters. There is no chemical database, but some chemical properties are available in the user manual.



<span id="page-23-0"></span>**Fig. 6** Wind speed profile according to the observations results of JR II 2015 and simulations results of sSLAB and SLAB-M models [[27](#page-27-3)]

The model does not generate graphical output and automatically sends tabular results to a printer file. These results include input data, instantaneous spatially average cloudiness parameters, time-averaged cloudiness parameters, and timeaveraged concentration values at the plume centerline and five off-centerline distances at four user-defined altitudes and the plume height.

*CHARM model,* or "Chemical Hazard Assessment and Risk Management," is a general model. TNO-Wageningen Marine Research helped to develop it in the context of OSPAR [\[28](#page-27-4)].

Risk assessment of the use and discharge of chemicals from offshore oil and gas platforms is carried out based on information from the HOCNF (Harmonized Offshore Chemical Notification Format). The model can be used for exploration, drilling, and production stages.

The list of equations of the CHARM model is presented in the appendices of the user manual [[29\]](#page-27-5).

#### *HEGADAS-5 model*

HEGADAS-5 software from Shell HEGADAS [[30\]](#page-27-6) is based on the steady-state model. The new model is based on a generalized concentration similarity profile. It is formulated to provide improved predictions of the vertical variation of concentrations. This profile is expressed regarding ground-level central concentration and vertical/cross-dispersion parameters. A crosswind propagation equation incorporating gravity-propagating collapse and generalized crosswind diffusion law is formulated to improve predicted cloud width. A new thermodynamic model is developed to provide HF dispersion in addition to ideal gases. New capabilities in HEGADAS were validated based on a wide range of experimental data.

#### *AFTOX model*

AFTOX computer model was developed and approved for use by the Air Weather Service in 1988 [[31\]](#page-27-7). AFTOX is a Gaussian layer dispersion model for uniform terrain and wind conditions. It will handle continuous or instantaneous releases, liquid or gas, elevated or surface releases from a point or local source. AFTOX 14.0 represents an updated version based on user feedback after two years of operating the model in the field. Changes make the program more user-friendly and improve it technically.

#### **6 Conclusions**

A large number of dangerous toxic substances are produced, stored, and transported in modern industry. However, emergencies may occur during various adverse circumstances. They are accompanied by the release of dangerous gaseous chemicals into the environment. Their spread threatens the life and health of the service personnel of enterprises and the population in the surrounding area. Analysis showed that

these gases form clouds heavier than air when accidentally released into the atmosphere. Heavy gas clouds have negative buoyancy. It affects their behavior relative to floating or neutrally polluted clouds and changes them. This is due to an additional gravitational flow, wind shear at the boundaries of heavy gas clouds, and turbulent discharge.

Empirical, engineering, and computational hydrodynamic (research) models of heavy gas dispersion are considered. Their advantages and disadvantages are shown. These models differ in complexity and mathematical description.

Examples of the work of research models, namely DEGADIS, ADAM, HGSYSTEM, SLAB, CHARM, HEGADAS-5, and AFTOX, are described and demonstrated. Their use allows simulation of consequences of the release (spill) of dangerous substances during accidents, investigation of characteristics of the influence of input factors on the process of spreading heavy gases in the environment, visibility increasing of the forecasting process of the consequences of accidents at chemically hazardous objects and transport by visualizing the calculation process and forecasting results.

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