DISPERSION MODELING FOR REGULATORY APPLICATIONS

by

Gligor KANEVCE and Ljubica KANEVCE

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Air quality simulation models are extensively used in assessing the impacts of combustion plants. A wide variety of models are available. In order to recommend the most appropriate air quality modeling technique that should be incorporated into a standard regulatory framework in the Republic of Macedonia the performances of three Gaussian-plume atmospheric dispersion models, ADMS 3, OML, and ISCST3 have been analysed. The models have been tested against the ground level measurements of the daily mean SO₂ concentrations obtained at the four locations around the Thermal Power Plant of Bitola. Two experimental campaigns have been performed. The three model results and the measurements at the presented locations for 365 days in the year are compared. An analysis of the obtained results is presented in the paper as well.

The meteorological preprocessor MADAM_MP has been used to provide the required boundary layer parameters for estimation of the transport and diffusion of pollutants released from the stacks. Using the MADAM_MP a year of hourly values for the mixing height, Monin-Obukhov length, surface friction velocity, sensible heat flux, and Pasquill's stability class, have been calculated from the available meteorological data set. The approach and the main equations for the boundary layer parameters estimation are presented in this paper.

Key words: atmospheric dispersion, MADAM_MP, OML, ADMS 3, ISCST3

Introduction

Air quality modeling is an essential tool for most air pollution studies. Models can be divided into physical (wind tunnel, water tank) and mathematical types. In air quality legislation the mathematical models are most advantageous. Consequently, they are analysed in this paper. They are particularly valuable for assessing the impacts of discharges from new activities and for estimating the likely changes as a result of process modifications. The mathematical models are a unique tool for:

- selecting locations and determining appropriate stack heights of new facilities (future sources of pollutants), in order to minimize their environmental impacts,
- managing existing emissions determining the maximum allowable emission rates that will meet fixed air quality standards,
- designing ambient air monitoring networks,

- saving cost and time over monitoring; modeling costs are a fraction of monitoring costs and a simulation of annual or multi-year periods may only take a few hours or days to assess,
- assessing responsibility for existing air pollution levels by evaluating source-receptor relationships, and
- forecasting pollution episodes.

In general, the models require two types of data inputs: information on the source or sources including pollutant emission rates, and meteorological data. The models then simulate mathematically the pollutant's transport and dispersion, and its chemical and physical transformations and removal processes. The models output is air pollutant concentration, for a particular time period, usually at specific receptor locations. The phenomena analysed in different types of air pollution problems are [1, 2]:

- local problems: short-range transport up to 20 km from the source. Identify the area in which the maximum ground-level impact of primary pollutants from an elevated source such as a power plant, factory, waste disposal site, and so on, is generally found;
- intermediate transport, between 10 and 100 km. In this area chemical reactions become important and must be taken into account. These problems include urban air pollution resulting from a variety of urban sources, and are often referred to as urban air pollution, examples of which are urban smog and haze;
- long-range transport, between 100 and 10000 km. The area in which large-scale meteorological effects and deposition and transformation rates play key roles. These types of air pollution problems are referred to as regional or interregional pollution. Examples are transport of sulphur and nitrogen oxides from major industrial areas to other regions where they are washed out of the air as acid precipitation;
- global effects; i. e., phenomena affecting the entire earth atmosphere. The best--known examples are global warming due to CO_2 and other greenhouse gases accumulation and the stratospheric ozone holes.

Modeling of short-range transport is analysed in this paper. Small-scale motions and processes occurring in the lowest layer of the atmosphere, called the planetary boundary layer or the atmospheric boundary layer or simply the boundary layer, essentially determine short-range dispersion of pollutants released from near-surface sources. The boundary layer is formed as a consequence of interactions between the atmosphere and the underlying land or water surface over short time scales ranging from one hour to one day. The physical and thermal properties of the underlying surface, in conjunction with the dynamics and thermodynamics of the lower atmosphere (troposphere), determine the planetary boundary layer structure including its depth, wind and temperature distributions, transport, mixing and diffusion properties, and energy dissipation. The boundary layer height is quite variable in both time and space, ranging from several tens of meters to a few kilometers. It is commonly referred to as the mixing height because pollutants released from near-surface sources are quickly mixed up to the top of the boundary layer and are usually confined to the boundary layer due to lack of mixing in the inversion layer above. Air quality legislation (or lack of it) has affected the development of air pollution modeling techniques in different countries. The continuing development of new atmospheric dispersion models all over the world causes some confusion in the application for regulatory purposes in the countries without its own Guideline on Air Quality Models, such as Republic of Macedonia. Accordingly, there is a need for consistency in the application of air quality models for regulatory purposes. In order to recommend the most appropriate air quality modeling technique that should be incorporated into a standard regulatory framework in the Republic of Macedonia, the short-range air dispersion model MADAM (Macedonian Air Dispersion Advanced Model) is being developed. In the present stage, the MADAM is intended for the air quality impact analysis of the continuous, elevated point sources, such as thermal power stacks, in rural, simple terrain. The model includes two modules: a meteorological data process module, and a dispersion calculation module. The Meteorological Preprocessor MADAM_MP provides a standard method of obtaining the required boundary layer parameters for the dispersion calculation module from a sequential hourly record of standard synoptic surface data.

Parameterisation of the boundary layer

Meteorology is fundamental for the dispersion of pollutants because it is the primary factor determining the diluting effect of the atmosphere. Therefore, the quality of a dispersion model strongly depends on the quality of its meteorological inputs. Since all the desired meteorological parameters are not usually measured at the location and time of release of the dispersion to be modelled, some method of estimating the boundary layer parameters must be used in dispersion applications. Although the gradient-transport theories, as well as the more sophisticated theories, are used in applications to air pollution meteorology and dispersion, the similarity theory based on dimensional analysis is still the most widely used for determination of the boundary layer structure and its thickness, wind and temperature distributions, transport, mixing and diffusion properties. There are few similarity theories in use. For the more frequently encountered stratified boundary layer, the Monin-Obukhov similarity theory has been widely accepted. It is based on the hypothesis that mean gradients and turbulence characteristics of the stratified surface layer depend only on the height z, the kinematic surface shear stress τ_0/ρ , the kinematic heat flux at the surface $H/\rho c_p$, and the buoyancy variable g/T, where T, ρ and c_n are the temperature, density, and specific heat capacity of the air, respectively. This leads to the following parameters of the Monin-Obukhov similarity theory:

- friction velocity:

$$u^* \quad \sqrt{\frac{\tau_0}{\rho}} \tag{1}$$

- friction temperature:

$$\theta^* = \frac{H}{\rho c_p u^*} \tag{2}$$

143

- height above surface:

(3)

- buoyancy (Monin-Obukhov) length:

$$L = \frac{\sqrt{(\tau_0 / \rho)^3}}{k \frac{g}{T} \frac{H}{\rho c_n}} = \frac{u^{*2}}{k \frac{g}{T} \theta^*}$$
(4)

In the different regions of the boundary layer different mechanisms are important in generating turbulence. These are:

Z

- surface heating or, convectively generated turbulence. The convective eddies increase in energy as they rise through the boundary layer,
- turbulence mechanically generated by shearing at the surface, and
- local shear at the top of the boundary layer as a weak source of turbulence.

The Monin-Obukhov length is a measure of the depth of the near-surface layer in which shear effects are likely to be significant under any stability condition. In unstable or convective conditions, the Monin-Obukhov length is negative. Then, the magnitude of the length is a measure of the height above the ground above which convective turbulence that is, turbulent motions caused by convective motions, is more important than mechanical turbulence generated by friction at the earth's surface. In stable conditions the Monin-Obukhov length is positive. Then it is a measure of the height above the ground above which vertical turbulent motion is greatly inhibited by the stable stratification.

The ratio of the two length scales, z/L, is the Monin-Obukhov stability parameter. Additionally, according to the mixed-layer similarity theory, the boundary layer stability is defined in terms of the ratio z/h, where h is the boundary layer height. The two previous stability parameters yield to a third one, h/L. The parameters, z/L and h/L, supersedes the Pasquill-Gifford formulation, and differs crucially from the Pasquill formulation in allowing the variation of boundary layer properties with height to be included. Figure 1 [3] shows the different regions of the boundary layer in terms of the parameters h/L and z (in the calculations z/L is used instead of z).

For comparison, fig. 1 also shows the Pasquill-Gifford stability categories corresponding approximately to ranges of h/L. It can be seen that the Pasquill-Gifford stability classes (A-G) are not simple functions of h/L.

In the MADAM_MP it is assumed that the boundary layer is self-similar for a given value of h/L. Three stability categories are classified [3]:

_	stable	h/L	1.0
_	neutral	-0.3	h/L < 1.0
_	convective	h/L < -0.3	

The boundary layer parameters are calculated from the standard synoptic surface data applying the van Ulden and Holtslag approach [4] that is based on the Monin-Obukhov similarity theory. The sensible heat flux, the Monin-Obukhov length, the surface friction velocity, the mixing height, and the convective velocity scale are calculated by the MADAM Meteorological Preprocessor.



Kanevce, G., Kanevce, Lj.: Dispersion Modeling for Regulatory Applications

Figure 1. Variation of Monin-Obukhov length and boundary layer height with atmospheric stability

The sensible heat flux, H, during daytime conditions is obtained from the energy balance at the earth's surface based on the Holtslag – van Ulden scheme [5]:

$$H = \frac{(1 - c_g)R_N}{1 - \frac{1}{B_g}}$$
(5)

where R_N is the net radiation, c_g is the fraction of the net radiation absorbed at the ground and B_o is the Bowen ratio.

The equations for the surface friction velocity, u^* :

$$u^* \quad \frac{kU_r}{\ln \frac{z_a}{z_0} \quad \Psi_m \frac{z_a}{L} \quad \Psi_m \frac{z_0}{L}} \tag{6}$$

and the Monin-Obukhov length, L

$$L = \frac{\rho c_p T u^{*3}}{k g H} \tag{7}$$

145

are iterated over u^* and L until the desired accuracy of L is reached. Here, U_r is the wind velocity at the anemometer height z_a , k (= 0.4) is the von Karman constant and z_0 is the surface roughness. The stability-dependent similarity function is:

$$\Psi_{\rm m} \frac{z}{L} = 2\ln \frac{1}{2} \frac{\chi}{2} = \ln \frac{1}{2} \frac{\chi^2}{2} = 2\arctan \chi = \frac{\pi}{2}$$
(8)

$$\chi = \sqrt[4]{1 - \frac{16z}{L}} \tag{9}$$

At night, the approach outlined by Hanna and Paine [6] is used to calculate the friction velocity, heat flux, and Monin-Obukhov length.

The friction velocity is calculated from:

$$u^* \quad \frac{C_D U_r}{2} \quad 1 \quad \sqrt{1 \quad \frac{4u_0^2}{C_D U_r^2}} \tag{10}$$

where

$$u_0 \quad \sqrt{\frac{4.7z_a g \theta^*}{T}} \tag{11}$$

and the drag coefficient, C_D

$$C_D = \frac{k}{\ln \frac{z_a}{z_0}} \tag{12}$$

The friction temperature, θ^* is:

$$\theta^* = 0.09(1 - 0.5N^2) \tag{13}$$

where *N* is the cloud cover.

Sensible heat flux is determined from eq. (2):

$$H = -\rho c_p u^* \theta^* \tag{14}$$

and the Monin-Obukhov length from eq. (7).

For wind velocities less than the value that provide real solutions, a slightly different approach is used.

The mixing height in stable and neutral conditions is calculated by the most popular diagnostic equations based on the equation for the Ekman-layer depth.

In stable conditions the mixing height is given by:

$$\frac{h}{L} = \frac{1}{3.8} \sqrt{1 \frac{2.28u^*}{fL}}$$
(15)

146

and, in neutral conditions by:

$$h \quad \frac{0.3u^*}{f} \tag{16}$$

where *f* is the Coriolis parameter.

In unstable conditions, evolution of the mixing height is determined by pair of first order ordinary differential equations [7-9]:

$$\frac{\mathrm{d}h}{\mathrm{d}t} \quad \frac{s}{\Delta\theta} \tag{17}$$

$$\frac{\mathrm{d}\Delta\theta}{\mathrm{d}t} \quad \frac{\gamma_{\theta}s}{\Delta\theta} \quad \frac{H}{\rho c_p h} \quad \frac{s}{h} \tag{18}$$

where,

$$s \quad \frac{02H}{\rho c_n} \quad \frac{5u^{*3}T}{gh} \tag{19}$$

 $\Delta\theta$ is the discontinuous potential temperature jump across the inversion base, and γ_{θ} , is the rate of increase of potential temperature with height above the boundary layer. The Runge-Kutta-Fehlberg integration method is used for the numerical solution of the eq. (17) and (18).

Dispersion models in regulatory applications

Although new types of dispersion models are now beginning to enter the regulatory arena, such as CALPUFF or TAPM [10, 11], the Gaussian-plume models are still commonly used in assessing the impacts of existing and proposed sources of air pollution on local and urban air quality, particularly for regulatory applications. The steady-state Gaussian-plume models are based on the mathematical approximation of plume behaviour and are the easiest models to use. They incorporate a simplistic description of the dispersion process, and some fundamental assumptions are made that may not accurately reflect reality. However, the assumptions, errors and uncertainties of these models are generally well understood. So, even with these limitations, this type of model can provide reasonable results when used appropriately. The primary justification for the use of Gaussian diffusion models in regulatory applications comes from their evaluation and validation against experimental diffusion data.

The Gaussian-plume formula is derived assuming "steady-state" conditions. The steady-state Gaussian-plume models calculate concentrations for each hour from an emission rate and meteorological conditions that are uniform across the modeling domain. Thus, they simulate hourly-average concentrations. Still they are time varying, changing from hour to hour. The term "steady-state" should not be taken to mean that conditions are steady from hour to hour. The Gaussian-plume formula for calculating the concentration of pollutant at downwind distance, x, crosswind distance, y, and height above ground, z, for a continuous point source of strength, M, in a uniform flow with homogeneous turbulence and mean wind velocity at stack height, U_s , can be expressed as:

$$C(x, y, z) \quad \frac{M}{2\pi\sigma_v\sigma_z U_s} \exp - \frac{y^2}{2\sigma_v^2} V \tag{20}$$

where, σ_y and σ_z are standard deviations of lateral and vertical concentration distribution, or, the Gaussian plume dispersion parameters. The plume formula has the mean wind velocity in the denominator and hence breaks down in calm conditions. It is usual to specify a minimum allowable wind velocity for the model.

The vertical term:

$$V = \exp \frac{(z H_{\rm ef} 2nh)^2}{2\sigma_z^2} \exp \frac{(z H_{\rm ef} 2nh)^2}{2\sigma_z^2} \quad n = 0, 1, 2, \dots (21)$$

accounts for the vertical distribution of the Gaussian plume. It includes the effects of source elevation, $H_{\rm eff}$, receptor elevation, z, and limited mixing in the boundary layer of height, h. The series term in eq. (21) accounts for multiple reflections of the plume from the ground and at the top of the boundary layer. In the usual practice the terms up to 4 are taken in to the calculations. The effective source height, $H_{\rm eff}$, is the sum of the stack height and plume rise. The plume rise is commonly modelled by methods proposed by Briggs [12, 13] supplemented by a number of extensions.

In developing the MADAM the performances of three very popular atmospheric dispersion models, ADMS 3, OML, and ISCST3 have been analysed.

ADMS 3 is a quasi-Gaussian model of dispersion in the atmosphere of passive, buoyant or slightly dense, continuous or finite duration releases from single or multiple sources which may be point, area or line sources [3]. The model uses an up to date parameterisation of the boundary layer structure based on the Monin-Obukhov length L, and the boundary layer height h. The concentration distributions are Gaussian in stable and neutral conditions, but the vertical distribution is non-Gaussian in convective conditions to take account of the skewed structure of the vertical component of the turbulence. The plume spread depends on the local wind velocity and turbulence and thus depends on plume height. The meteorological pre-processor calculates the required boundary layer parameters from a variety of input data. Meteorological data may be raw, hourly averaged values, or statistically analysed data.

The OML is a modern Gaussian plume model [14, 15]. It belongs to the same class of models as ADMS. It does not use traditional discrete Pasquill stability categories, but instead describes dispersion processes in terms of basic boundary-layer scaling parameters, such as friction velocity, Monin-Obukhov length, and the convective velocity scale. The OML model is intended to be used for distances up to about 20 km from the source. The source is typically one or more stacks, and possibly also area sources. Typi-

cally, the OML model is applied for regulatory purposes. In particular, it is the recommended model to be used for environmental impact assessments when new industrial sources are planned in Denmark. The model requires information on emission and meteorology on an hourly basis.

As a representative of the models that describe the boundary layer structure in terms of the Pasquill-Gifford Stability Category, the Industrial Source Complex Short Term (ISCST3) model has been analysed [16]. The ISC Short Term model uses a steady-state Gaussian plume equation to model emissions from point sources, such as stacks and isolated vents. The ISC Short Term model accepts hourly meteorological data records to define the conditions for plume rise, transport, diffusion, and deposition. The model estimates the concentration or deposition value for each source and receptor combination for each hour of input meteorology, and calculates user-selected short-term averages. The user also has the option of selecting averages for the entire period of input meteorology. ISCST3 is a US EPA regulatory model. Formally, in 2000, AERMOD [17] was proposed by the US EPA as a replacement for ISCST3. However, this status has not yet been achieved.

Results and discussion

The performances of the atmospheric dispersion models ADMS 3, OML, and ISCST3 where tested against the ground level measurements of the daily mean SO_2 concentration obtained at the four locations around the Bitola Thermal Power Plant. This power plant is located nearly in the middle of the 70 km long and 15 km wide Pelagonia valley. It is a 675 MW coal fired plant with two stacks. They are located at a distance of 50 m from each other. The stacks height is 250 m and the stacks diameter is 8.4 m.

Two experimental campaigns were performed. The first was in the period January 1st to December 31st of 1998 and the second one from the February 1st 2001 to the January 31st 2002. The obtained results were similar. The emission rates of SO₂ were 1072 and 2144 g/s and the exit velocities 12.1 and 24.2 m/s for the stack 1 and stack 2, respectively. The exit temperature was 448 K.

A year of hourly surface weather data, obtained during the experimental campaigns from the Bitola Meteorological Station located about 10 km east and MS Kremenica located about 12 km south of the power plant have been used. From the available surface measurements, a data set has been created, which includes hourly values for wind velocity, wind direction, atmospheric pressure, temperature, relative humidity, observed total cloud cover, presence of cirrus clouds, presence of precipitation, presence of snow, and observed cloud ceiling heights.

The meteorological preprocessor MADAM_MP has been used to provide the required boundary layer parameters for estimation of the transport and diffusion of pollutants released from the stacks. Using the MADAM_MP a year of hourly values for the mixing height, h, Monin-Obukhov length, L, surface friction velocity, u^* , sensible heat flux, F, and Pasquill's stability class (PSC) have been calculated from the available meteorological data set.

Figure 2 presents wind velocity and a Pasqill stability class frequency bar chart created from the output of MADAM_MP. It can be seen that the meteorological situation is characterized by a very high percentage of wind velocities below 1 m/s including the calm conditions. It can be also seen that D and E to G stability classes, or neutral and stable meteorological conditions prevail.



Figure 2. Wind velocity and Pasquill stability class frequency chart

Figure 3 illustrates evolution of the mixing height, h, during the winter, summer, and windy autumn day, estimated with the MADAM MP.

Frequency distribution for the estimated mixing heights is presented on fig. 4. It can be seen that more than 50% of the estimated mixing heights are lower than the stacks height of 250 m.



Figure 3. Evolution of the mixing height during selected days

Using the dispersion models ADMS 3, OML, and ISCST3 the ground level daily mean SO₂ concentration at the four locations were calculated. The coordinates (x, y, [m]) of the receptor locations, relative to the stack1 are: Biljanik (473, -2147), Dedebalci (-17, 6238), Gneotino (-414, -8092), and Ribarci (-1407, -4564).

OML has been adapted for running without mixing height observations input by the authors of the model. Daily average concentration values of SO_2 have been calculated by a year of hourly surface weather data, running the model day by day.

The Air Dispersion Model ADMS 3 has been run for 365 sets of meteorological data to provide 365 daily mean ground level concentrations at four specified locations. One set of meteorological data has



Figure 4. Frequency distribution for mixing heights

been used to obtain one mean ground level concentration for sequential calculations, which simulate a 24-hour period [3].

In running ISCST3 for our study, the regulatory default option [16] and a sequential hourly record of meteorological variables generated by the MADAM met preprocessor have been used.

The results of the comparison between predicted concentrations and measurements are presented in fig. 5. The figure shows a Quantile-Quantile plot generated using observed and predicted daily mean ground level concentrations at the four specified locations. In the Quantile-Quantile plot the ranked values are compared. The ISCST3 and ADMS 3 were used for the ground level daily mean SO₂ concentration prediction for both of the performed experimental campaigns and OML only for the first one.



Figure 5. Comparison of measured and computed daily SO₂ concentration for TPP of Bitola data Quantile-Quantile plot

A summary of discussion is given below:

- Measured and calculated daily mean concentrations have low values, below 50 g/m³, with high percentage of very low values, below 20 g/m³.
- In many cases all three models gives zero calculated concentrations, which can be explained with a high percentage of mixing heights lower than heights of stacks.
- ISCST3 and ADMS give results, which are comparable with measurements and follow the trend of changes. Differences between measurements and model values, in the cases where the measurements are very small, *i. e.*, less than 10 g/m³ while model's predictions are equal to zero, can be partly explained by background concentrations.
- OML model also follows the trend, but gives lower results than measurements. An explanation of such behaviour is that the OML meteorological pre-processor, beside the hourly meteorological measurements from a synoptic surface station, has typically as input twice-daily vertical profiles of temperature from a nearby radiosonde station. In our application only surface measurements were available.

Conclusions

The needs and advantages of the mathematical models in the air quality legislation are underlined in the paper.

The MADAM Meteorological Preprocessor (MADAM_MP) intended for application in the regulatory setting in the Republic of Macedonia, where only standard synoptic surface meteorological data are available is presented. In this paper the approach and the main equations for the boundary layer parameters estimation are presented.

The performances of three Gaussian-plume atmospheric dispersion models ADMS 3, ISCST3, and OML have been analysed. The models were tested against the ground level measurements of the daily mean SO_2 concentration obtained at the four locations around the Bitola Thermal Power Plant. An analysis of the obtained results is presented in the paper as well.

The required boundary layer parameters for estimation of the transport and diffusion of pollutants released from the stacks were estimated. Using the MADAM_MP a year of hourly values for the mixing height, Monin-Obukhov length, surface friction velocity, sensible heat flux and Pasquill's stability class have been calculated from the created meteorological data set.

The main characteristics of the available meteorological data are the high percentage of wind velocities below 1 m/s and the lack of mixing height or other vertical profile measurements. The main characteristic, of both, the measured and predicted daily SO_2 concentration values, is that they are small, less than 50 g/m³, with a high percentage of very small values, below 20 g/m³.

Despite the lack of mixing height measurements, very low wind velocity values, and very low ground level SO₂ concentrations, the results of all three models were good. Thus, it can be concluded that OML, ADMS 3, and ISCST3, after some additional analyses, can be used for development of the Macedonian Regulatory Model.

Kanevce, G., Kanevce, Lj.: Dispersion Modeling for Regulatory Applications

Nomenclature

- $B_{\rm o}$ - Bowen ratio, [-]
- concentration, [kgm⁻³] C
- C_D - drag coefficient, [-]
- fraction of net radiation absorbed at the ground, [-] C_g
- specific heat capacity of air, [JK⁻¹kg⁻¹]
 Coriolis parameter, [s⁻¹] c_p
- f
- acceleration due to gravity, [ms⁻²] g
- sensible heat flux at the surface, $[Wm^{-2}]$ H
- $H_{\rm ef}$ - effective source height, [m]
- mixing height, [m] h
- the von Karman constant, [-] k
- L - Monin-Obukhov length, [m]
- М - emission rate, [kgs⁻¹]
- fraction of cloud cover, [-] Ν
- R_N - net radiation, [Wm⁻²]
- Т - temperature, [K]
- time, [s]t
- air temperature at the reference state, [K] T_0
- U_r - mean wind velocity at the anemometer height, [ms⁻¹]
- mean wind velocity at stack height, $[ms^{-1}]$ U_{s}
- u^* - friction velocity, $[ms^{-1}]$
- x, y, z coordinates, [m]
- anemometer height, [m] Z_a
- surface roughness, [m] Z_0

Greec letters

- γ_{θ} vertical potential temperature gradient, [Km⁻¹]
- ρ density, [kgm⁻³]
- σ_v standard deviation of lateral concentration distribution, [m]
- σ_z standard deviation of vertical concentration distribution, [m]
- $\tau_{\rm o}~-$ surface shear stress, $[\rm Nm^{-2}]$
- θ potential temperature, [K]
- θ^* friction temperature, [K]
- $\Delta \theta$ discontinuous temperature jump across inversion base, [K]
- Ψ_m stability dependent similarity function, [–]

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Authors' address:

G. Kanevce,

Macedonian Academy of Sciences and Arts Skopje, Macedonia

Lj. Kanevce Faculty of Technical Sciences, St. Kliment Ohridski University Bitola, Macedonia

Coresponding author (Lj. Kanevce): E-mail: kanevce@osi.net.mk

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