

Czech Technical University in Prague
Faculty of Mechanical Engineering

Summary of Ph.D. Thesis

**NUMERICAL SOLUTION OF FLOW
AND POLLUTION DISPERSION
IN ATMOSPHERIC BOUNDARY LAYER**

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Summary

This work deals with the mathematical and numerical modelling of flow and pollution dispersion in atmospheric boundary layer.

Starting from general formulation of conservation laws governing the flow dynamics of general fluid, the series of approximations is developed. The dimensional analysis of the basic governing systems is presented as a basic tool for the development of simplified models. The range of applicability of these simple models is discussed.

Selected models are studied in more detail and suitable numerical methods are proposed for their solution. The corresponding finite-volume and finite-difference schemes are developed and described in detail. Deeper analysis of the semi-implicit scheme, used for the solution of the Boussinesq approximation, is performed with special focus on numerical dissipation and dispersion properties of the scheme.

The latest generation model based on Boussinesq approximation is used in numerical experiments in order to validate the method. The simple flows and pollution dispersion over 2D and 3D sinusoidal hills are studied. Results of computations are compared with experimental or numerical data of other authors as they have been published in available literature. Based on this numerical experience the model is applied to the real terrain, large scale circulation in mediterranean coastal area. The functionality of the method is extended for the flow over real orography, with the use of real (i.e. measured) boundary data and for unsteady boundary conditions.

Throughout of the thesis not only the work that has been done is presented, but also some ways of future research and extension of the project are proposed and discussed.

Shrnutí

Tato práce se zabývá matematickým a numerickým modelováním proudění a šíření znečištění v mezní vrstvě atmosféry.

Vycházejí z formulace bilančních rovnic, které popisují proudění tekutiny, je odvozena posloupnost aproximací těchto základních rovnic. K odvození zjednodušených modelů je použita rozměrová analýza původního, kompletního modelu proudění. Spolu s odvozením jsou diskutovány i hranice použitelnosti zjednodušených modelů.

Vybrané modely jsou studovány detailněji a jsou pro ně navrženy numerické metody vhodné k jejich řešení. Zvolená schemata ve formě konečných diferencí a konečných objemů jsou detailně odvozena a popsána. Je provedena hlubší analýza semi-implicitního schematu použitého pro řešení Boussinesquovy aproximace. Zvláštní důraz je kladen na studium vlivu numerické difuze a disperze schemat.

Poslední generace modelu, založená na Boussinesquově aproximaci, je použita k numerickým experimentům s cílem ověřit použitelnost zvolené metodiky řešení. Je studováno proudění a šíření znečištění v blízkosti dvoj- a troj-rozměrných kopců sinusoidálního průřezu. Výsledky výpočtů jsou srovnávány s experimentálními a numerickými daty publikovanými jinými autory v dostupné literatuře. Na základě zkušeností s těmito jednoduchými případy, je metoda použita k řešení proudění v oblasti středomořského pobřeží. Použitelnost metody je rozšířena pro případy proudění přes reálnou orografii, s použitím reálně naměřených dat a pro užití nestacionárních okrajových podmínek.

V rámci celé práce jsou prezentovány a diskutovány nejenom výsledky dosavadního vývoje, ale i možné směry dalšího výzkumu a kroky vedoucí k rozšíření stávajícího a vývoji nového modelu pro popisovanou třídu problémů.

List of symbols

Alphanumeric symbols:

a	...	advection velocity
C^i	...	concentration of i -th pollutant
f_c	...	Coriolis parameter
g	...	gravity acceleration
H	...	height of the hill
K	...	turbulent diffusion coefficient
L_1	...	length of the hill (see Fig. 3)
p	...	pressure
t	...	time
u	...	x component of velocity
v	...	y component of velocity
w	...	z component of velocity
x	...	x -coordinate
y	...	y -coordinate
z	...	z -coordinate

Greek symbols:

Δt	...	time step
Δx	...	space step
ϵ_2, ϵ_4	...	artificial viscosity coefficients
γ	...	parameter $\gamma = a\Delta t/\Delta x$
ρ	...	fluid density
ρ_0	...	background fluid density
σ_C	...	Prandtl's number for concentration
σ_Θ	...	Prandtl's number for potential temperature
Θ	...	potential temperature

Subscripts:

\cdot_0	...	background variable
\cdot_G	...	geostrophic (e.g. velocity)
\cdot_i	...	mesh space index
\cdot_t	...	time derivative
\cdot_x	...	x -derivative
\cdot_y	...	y -derivative
\cdot_z	...	z -derivative

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1 Introduction

The air pollution resulting from the rapid industrialization has become a serious public environmental problem. The accurate evaluation of environmental impact has received an increased attention during the past decades and is now one of the key points in further development of any industrial region. There are two basic possible approaches to this problem.

The first one is the *physical modelling* that involves the use of geometrically scaled-down model in a wind-tunnel. However it is nearly impossible to satisfy all the similarity requirements in this case because of large scaling factors (1/500–1/1000) and complexity of atmospheric conditions.

The second method is based on *mathematical modelling*. The classical pollution models deal with the Gaussian plume model. However the Gaussian plume models applicability is restricted to the pollution dispersion over a flat terrain. In the case of flow over complex topography the predicted results could contain unacceptable errors. The pollution dispersion in complex terrain is mainly influenced by the local flow field and thermal stability conditions. In this situation (where the analytical solution is not possible to obtain) the numerical methods based on solution of systems of partial differential equations could be employed.

According to the Prandtl's hypothesis the air in motion can be divided into "main flow", where viscosity plays a negligible role, and "boundary layer flow", where fluid friction is influential. The boundary layer is always close to a surface such as the surface of a planet. In literature it is possible to find many different definitions of *Atmospheric Boundary Layer* (ABL). Here are just few of them:

- The part of troposphere that is directly influenced by the presence of the earth's surface, and responds to surface forcing with a time scale of about an hour or less.
- The interface between the surface of the earth and the free atmosphere.
- The lowest one to two kilometers of the Earth's atmosphere in direct contact with the Earth's surface.
- The layer of air covering the earth, the thickness of which is determined by the height at which surface friction no longer affects the flow of wind.
- The part of lower troposphere in which physical, chemical and biological processes of the atmosphere are largely governed by the conditions of the underlying surface.

It is not just the wide range of definitions, that entitles us to take it that ABL is not a trivial system. There are some significant attributes of ABL modelling that urge us to develop special numerical methods for this case. We mention at this place just the most important properties of Atmospheric Boundary Layer:

- Anisotropic turbulence
- Large scale vorticity
- High Reynolds numbers flows
- Influence of Coriolis force
- Thermal stratification
- Large computational domains
- High resolution requirements
- Large time-scales of changes

2 State of the Art

These facts given above result in many contradictory requirements that is very difficult to satisfy by any mathematical (so as physical) model. In the field of mathematical modelling of the flow field there are used many more or less complex models. One wide class of models is based on linear-perturbation theory (mainly developed in 70's and 80's). The use of this approach is limited to the situations where the terrain is represented by smooth, moderate slope, low hills. Some details concerning such models can be found e.g. in papers *Mason & Sykes* [14], [3] or *Mason & King* [13], where also some basic experimental observations are presented. These models were finalized and summarized to form some type of "guidelines" for computing the flow parameters for simple terrain geometries. The extensive summary and review of these models so as measurements is given in *Taylor, Mason, & Bradley* [17] published in 1985. This simple "guideline" approach has been further improved and extended (in 90's) e.g. in the works *Miller & Davenport* [15] and *Weng, Taylor, & Walmsley* [18]. However these models can provide just a very limited information in the really complex terrain flows. The presence of steep hills often results in massive flow separation and recirculation. In such a case the guidelines will fail in the estimation of flow parameters. That is why the new generation of models started to dominate in this field during the past years (in 90's). These new models are based on the numerical simulations rather than on trying to estimate the flow characteristics. They are able to treat significantly more complex situations. The price we should pay for this qualitative jump, is the enormous increase of computational cost of such kind of simulations. Nevertheless with the increasing speed of computational tools, we have more and more possibilities to improve the numerical models at the level of physical parametrization so as at the stage of numerical solvers. That is why the tendency in current development is to use quite complex fluid mechanics models (such as the Navier-Stokes equations are) rather than to apply some of the classical simple approximations. Many works dealing this subject were published in the past years. Let's mention here e.g. the works *Ferreira, Lopes, Viegas, & Sousa* [9], *Kim, Lee, Lim, & Kyong* [12] and *Carpenter & Locke* [5]. These models can provide more detailed information about the flow field, but they need to be calibrated using some (wind tunnel or full scale) experimental data. That is why the comparison of physical and numerical data can be found in most of the above mentioned papers.

Specific area of atmospheric simulations is the pollution dispersion problematics. The classical analytical methods are based on the available exact solutions for passive pollutant dispersion over a flat surface. These Gaussian plume models have limited applicability in complex terrain and they cannot be easily extended for such cases. That is why also here the numerical methods, based on solution of partial differential equations, are now widely explored. Typical examples of such approach can be found e.g. in *Casro & Apsley* [6] and *Castro & Apsley* [7]. A wind tunnel studies of boundary layer dispersion were published e.g. in the papers *Gong* [11], *Arya, Capuano, & Fagen* [2] and *Crooks & Ramsay* [8].

The actual situation is now still favorable for simplified models at the scale of global or at least continental simulations. However the development of meso- and micro-scale models is more similar to the general computational fluid dynamics (CFD) evolution.

3 Objectives of the Work

The aim of this work is to establish a mathematical and numerical method for prediction of the atmospheric wind flow and the pollutant dispersion over complex terrain.

The following steps are taken to achieve the objectives of the present investigation:

I. The choice of mathematical model

This is the key point for the further investigation. The system must be general enough to be able to fully resolve the complex terrain phenomenology but should be also relatively easy to solve.

II. Development of numerical method and solver

In this step is necessary to chose numerical scheme that is accurate on one hand and simple, fast and easy to implement on the other hand.

III. Validation and application of presented method

To show the applicability and reliability of the method on simple test cases where the solution can be compared with the measurements or with numerical results obtained using another method.

The structure of the work

According to the above points the presented text can be divided into three main parts.

Part I.–Physics

Introduces the basics of physical parametrizations and models working in fluids with special focus on atmosphere. We start from formulating the basic set of conservation laws that are the most general principles that govern the physical processes in fluids. This system is then simplified in order to get a sequence of modells for specific situations. Some questions of the limited validity of these simplified models are discussed.

Part II.–Mathematics

Describes the numerical methods that can be (and are) used to solve the models formulated in the previous part. Some basic mathematical properties of the models and corresponding numerical schemes are discussed. The finite-difference semi-implicit scheme is described in more detail. The essential difficulties are pointed out and some improvement strategies are proposed.

Part III.–Application

Demonstrates the use of the models and solution methods described in the first two parts. Firstly some simple test computings are presented in order to validate the method on known wind tunnel data. The second set of numerical results shows the implementation of the numerical model for the real terrain problems. The specific problems connected with the use of numerical atmospheric models is discussed. At the very end of the work a real situation case is solved and the propositions for future model development are presented.

In addition to these three main parts, the work contains the **Appendix** where some auxiliary and supplementary material is presented.

4 The Review of Atmospheric Modelling Project

We have started with the numerical simulation of Atmospheric Boundary Layer flows in the 1996. In the first works we have used the simple 2D model based on incompressible Navier-Stokes equations. The system of governing equations was solved using explicit Mac-Cormack scheme in finite volume formulation.¹ In this simple model we have tested different types of artificial viscosity and different mesh configurations. Later we have implemented to our method some simple prototypes of eddy viscosity models. They were of similar type as the algebraic turbulence model later used in our models. *For references see² e.g. [1], [2] and [24].*

According to the experience with this simple 2D model, we have started in 1997 the development of first 3D method. In this case we have chosen the simplified governing system referred here as ABL approximation. This system we have solved using semi-implicit finite-difference scheme. The computational mesh and artificial viscosity terms were the 3D extensions of the previously used ones. Some comparative tests with the explicit finite-difference Mac Cormack scheme computations were performed. In this case we have for the first time used the algebraic turbulence model. The Coriolis effects for non-inertial coordinate system were also taken into account in this model. In 1998 we have implemented to this model the transport equations for passive pollutant and potential temperature. We have further studied the dispersion of pollutants from the elevated point sources. The influence of numerical and artificial viscosity was studied in the detail during the 1999. *For references see e.g. [11], [12] and [26].*

Equipped with the experience from the simplified 3D model we have started in 2000 to develop a new model. This time we have used the more complex Boussinesq approximation. The numerical solution has used the same semi-implicit finite-difference approximation as in previous model, however this time in time-marching artificial compressibility formulation. This model already includes some simplified treatment for stratified flows. The model equations and turbulent closure were modified in the corresponding way. In this model we have used all the successful features of the previous models, i.e. the mesh structure, numerical viscosity, discretization approach. With this last generation model we have started in 2001 the extensive validation and real-life simulation experiments³. *For references see e.g. [16], [17] and [23].*

All the numerical results presented in this work were obtained by this last generation model based on Boussinesq approximation. For older results including the comparisons of different models see the references listed in section 8.

¹Parallel work on the same model but with the use of different numerical scheme (Runge-Kutta multistage scheme) was performed by another member of our group – Luděk Beneš.

²The references of the type [XX] refer to published and unpublished works of the author of this thesis. The list of these publications is given in Section 8.

³The alternative model based on 3D RANS system was developed at the same type in our group by Luděk Beneš and Ivo Sládek. Some common comparative works were published. See the reference list.

5 Physics

The fluid flow can be described in the terms of invariants of motion i.e. by the means of “conservation laws” for certain essential quantities describing fluid in motion. Taking this as a cornerstone of development of mathematical model for fluid dynamics simulations, the governing system of equations for general fluid in motion should consists of the principles of conservation of mass, momentum and energy. In the case of Newtonian ideal fluid the governing system, consisting of the above mentioned conservation laws, is called Poisson-Stokes equations or more often *compressible Navier-Stokes equations*.

5.1 Development of simplified models

This system is the most general model for CFD simulations and its solution, even with the use of powerful computer tools, is still one of the most difficult tasks. That is why many simplified versions of this basic system were developed for the use in specific situations. Typical example of such reduced model is the system of *incompressible Navier-Stokes equations*.

According to scale of a problem we need to solve, some of the terms of minor importance can be neglected in momentum equations. Consider e.g. the u - momentum equation. Some of the classical models are summarized in the following table ⁴. Cases marked with • where the terms are considered.

	$\frac{\partial u}{\partial t}$	$u \frac{\partial u}{\partial x}$	$v \frac{\partial u}{\partial x}$	$w \frac{\partial u}{\partial x}$	$\frac{1}{\rho} \frac{\partial p}{\partial x}$	$f_c v$	$\frac{\partial}{\partial x} [K \frac{\partial u}{\partial x}]$	$\frac{\partial}{\partial y} [K \frac{\partial u}{\partial y}]$	$\frac{\partial}{\partial z} [K \frac{\partial u}{\partial z}]$
1.	•	•	•	•	•	•	•	•	•
2.	•	•	•	•	•				•
3.	•	•	•	•	•	•			
4.		•	•	•	•	•			
5.					•	•			
6.					•	•			•
7.					•				•

Table 1: Atmospheric flows approximations (According to *Brown* [4])

In the above table different rows correspond to different approximations as specified in the following summary:

1. Navier-Stokes equation, full system with Coriolis force, inside ABL

⁴The details can be found in *Brown* [4]

2. Prandtl equation, horizontal boundary layer in inertial coordinate system
3. Atmospheric flow outside (above) ABL
4. Steady atmospheric flow outside (above) ABL - gradient wind
5. Steady horizontally homogeneous flow above ABL - geostrophic wind
6. Ekman layer equations - steady, horizontally homogeneous ABL
7. Surface layer equations

5.2 Mathematical and numerical models for ABL flows problems

In our simulations we have used three different models. For the solution of each of them a suitable numerical method was chosen and corresponding computer code was developed. A brief summary of mathematical models used in our simulation is given here.

5.2.1 Reynolds averaged Navier-Stokes equations

The incompressible (with constant density) RANS equations in conservative form ^{5 6}:

$$u_x + v_y + w_z = 0 \quad (1)$$

$$u_t + (u^2 + p)_x + (uv)_y + (uw)_z = [Ku_x]_x + [Ku_y]_y + [Ku_z]_z + f_c v \quad (2)$$

$$v_t + (uv)_x + (v^2 + p)_y + (vw)_z = [Kv_x]_x + [Kv_y]_y + [Kv_z]_z - f_c u \quad (3)$$

$$w_t + (uw)_x + (vw)_y + (w^2 + p)_z = [Kw_x]_x + [Kw_y]_y + [Kw_z]_z \quad (4)$$

Here the hydrostatic part of pressure was removed (as in Boussinesq approximation) and the remaining deviation was normalized by density i.e. $p = p/\rho$. This system can be used for computation of turbulent incompressible atmospheric flows. No density- or temperature stratification is allowed.

5.2.2 Boussinesq approximation

The Boussinesq approximation in non-conservative form:

$$(\rho_0 u)_x + (\rho_0 v)_y + (\rho_0 w)_z = 0 \quad (5)$$

$$u_t + uu_x + vv_y + ww_z = -\frac{p''_x}{\rho_0} + \frac{1}{\rho_0} \left\{ [\rho_0 K u_x]_x + [\rho_0 K u_y]_y + [\rho_0 K u_z]_z \right\} + f_c v \quad (6)$$

$$v_t + uv_x + vv_y + vw_z = -\frac{p''_y}{\rho_0} + \frac{1}{\rho_0} \left\{ [\rho_0 K v_x]_x + [\rho_0 K v_y]_y + [\rho_0 K v_z]_z \right\} - f_c u \quad (7)$$

$$w_t + uw_x + vw_y + ww_z = -\frac{p''_z}{\rho_0} + \frac{1}{\rho_0} \left\{ [\rho_0 K w_x]_x + [\rho_0 K w_y]_y + [\rho_0 K w_z]_z \right\} - \frac{\Theta''}{\Theta_0} g \quad (8)$$

This system should be completed by the transport equation for potential temperature (except the thermally undisturbed case where $\Theta'' = 0$).

This system can be used for computation of weakly stratified turbulent atmospheric flows.

⁵We will no more use the overbar for Reynolds averaged quantities.

⁶The subscripts $_{txyz}$ will denote the partial derivatives with respect to time and x, y, z coordinates

5.2.3 ABL approximation

The non-conservative form of ABL approximation looks as follows:

$$u_x + v_y + w_z = 0 \quad (9)$$

$$u_t + uu_x + vv_y + ww_z = [Ku_z]_z + f_c(v - v_G) \quad (10)$$

$$v_t + uv_x + vv_y + wv_z = [Kv_z]_z - f_c(u - u_G) \quad (11)$$

This is the simplest of our models that can be used just for computation of incompressible, hydrostatic flows over almost flat terrain.

5.2.4 Transport equations

The same form as the momentum equations take also the transport equations for passive pollutants and the potential temperature dispersion. The non-conservative differential form looks as follows:

$$C_t^i + uC_x^i + vC_y^i + wC_z^i = \left[K \frac{C_x^i}{\sigma_{C^i}} \right]_x + \left[K \frac{C_y^i}{\sigma_{C^i}} \right]_y + \left[K \frac{C_z^i}{\sigma_{C^i}} \right]_z \quad (12)$$

$$\Theta_t + u\Theta_x + v\Theta_y + w\Theta_z = \left[K \frac{\Theta_x}{\sigma_\Theta} \right]_x + \left[K \frac{\Theta_y}{\sigma_\Theta} \right]_y + \left[K \frac{\Theta_z}{\sigma_\Theta} \right]_z \quad (13)$$

Here C^i is the concentration of i-th pollutant and σ denotes the turbulent Prandtl's number. Typically $\sigma = 0.74$. These equations can easily be transformed into conservative form (for the use with the model described in section 5.2.1) or simplified (to take the form of momentum equations from section 5.2.3).

5.3 Model characterization

The most general of the models we have used is the *Boussinesq approximation*. It is often presented and developed as a weakly-compressible extension of the incompressible Navier-Stokes model. Among variety of forms of this model used by different authors, we have chosen the one dealing with temperature rather than with the density variation. It is a common approach in boundary layer meteorology, where the temperature, as an easily measurable quantity, is taken as the cause for the density variation and stratification. In the special case of neutral stratification without temperature (and thus density) variation the system reduces to the incompressible Navier-Stokes system.

The *Navier-Stokes equations*, in the Reynolds-averaged version used here, is the classical choice for all the wind-tunnel scale numerical experiments, where no density- or temperature-variations are taken into account.

Further step in simplification is the *Atmospheric Boundary Layer approximation* which is based on hydrostatic and geostrophic assumptions together with the classical Prandtl's theory of boundary layer. That is why this system can only be used in case of very smooth terrain and indifferent thermal stratification. Otherwise some of the assumptions used to develop the model will be broken and the solution will become unphysical.

6 Mathematics

6.1 Numerical methods

Different numerical methods have been used to solve the above mentioned governing systems. Here is presented just the short summary of the numerical methods used:

- 1) **Reynolds averaged Navier-Stokes equations** (steady)
 - Artificial compressibility method (time-marching method)
 - Finite volume central space discretization
 - Explicit time integration
 - Artificial viscosity stabilization
- 2) **Boussinesq approximation** (steady)
 - Artificial compressibility method (time-marching method)
 - Finite difference central space discretization
 - Semi-implicit time discretization
 - Artificial viscosity stabilization
- 3) **ABL approximation**
 - Finite difference central space discretization
 - Semi-implicit time discretization
 - Artificial viscosity stabilization

The latest generation of our models is based on Boussinesq approximation solved by the semi-implicit finite-difference scheme. That is why this scheme is studied in a little bit more detail with special attempt to its diffusive and dispersive behavior.

6.2 Semi-implicit scheme

The combination of different asymmetric space discretization at time levels n and $n + 1$ allows us to construct finally the numerical scheme that is centered and second order in both space and time. The computational stencil is different for discretization at time level n and $n + 1$.

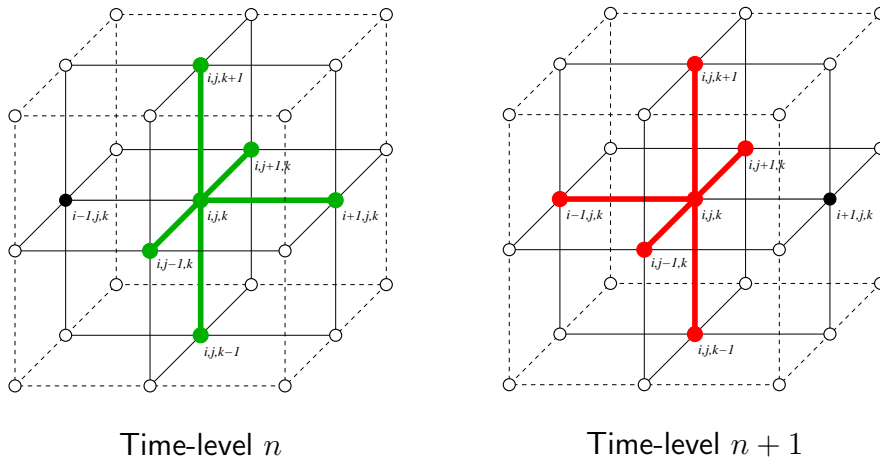


Figure 1: Computational stencil for semi-implicit FD scheme

Taking a closer look to the discretizations used in specific directions we see that the semi-implicit scheme we have used is in fact a combination of *Wendroff* type scheme in x direction, while for y and z directions the symmetric *Crank-Nicolson* discretization was employed. We start with a simple comparison of 1D modified equations (for the linear advection equation solution) for the above mentioned Wendroff and Crank-Nicolson schemes with some of the well known explicit schemes.

Scheme	Modified equation
Up-wind	$u_t + au_x = \frac{\Delta x}{2}(a - a^2\gamma)u_{xx}$
Lax-Wendroff	$u_t + au_x = -\frac{\Delta x^2}{6}(a - a^3\gamma^2)u_{xxx}$
Wendroff	$u_t + au_x = -\frac{\Delta x^2}{12}(2a + 3a^2\gamma + a^3\gamma^2)u_{xxx}$
Crank-Nicolson	$u_t + au_x = -\frac{\Delta x^2}{12}(2a + a^3\gamma^2)u_{xxx}$

Table 2: Modified equations

In the modified equations for Wendroff and Crank-Nicolson schemes are on the right-hand side just the terms with third order derivatives. These terms have dispersive character and they are the source of oscillations in the numerical solution. From the negative sign of coefficient before u_{xxx} we may conclude that the group velocity of oscillations is less than a and that is why the numerical solution oscillates just before the shock. (Compare with the Lax-Wendroff scheme.) There is no numerical diffusion present neither in the Wendroff nor in Crank-Nicolson scheme. It means that the numerical oscillations are not dumped like in the Up-wind scheme, where the strong numerical viscosity presented in the scheme guarantees the smoothness of solution. (But the Up-wind method is just first order accurate.) The higher frequency oscillations observed in the numerical solution using Wendroff and Crank-Nicolson scheme when compared with the Lax-Wendroff solution is due to the presence of numerical viscosity of fourth order (Term $-\epsilon u_{xxxx}$; $\epsilon > 0$ in higher order modified equation.) in the Lax-Wendroff scheme, which dumps the oscillations at smaller wavelengths.

The simplest way how to improve the quality of numerical solution using Wendroff and Crank-Nicolson schemes is to add some artificial viscosity into these schemes and to dump the numerical oscillations. It means the advection-diffusion equation (or viscous advection equation):

$$u_t + au_x = \epsilon_2 u_{xx} \quad \text{or better} \quad u_t + au_x = \epsilon_2 u_{xx} - \epsilon_4 u_{xxxx} \quad \epsilon_2, \epsilon_4 > 0 \quad (14)$$

will be solved instead of the original advection equation.

In the numerical solution it results in adding one more step in the solution algorithm.

First step - solution

$$\bar{U}^{n+1} = LU^n$$

Where the L represents the scheme dependent evolution operator of numerical method. (Or the shift operator from time level n to the time level $n + 1$.) The $U^n = \text{col}(u_0^n, u_1^n, \dots, u_{n_x-1}^n, u_{n_x}^n)$ is the vector of unknowns.

Second step - smoothing

$$U^{n+1} = \bar{U}^{n+1} + DU^n$$

There DU^n denotes an artificial viscosity term which operates at the time level n .

According to the modified equation analysis the following type of artificial viscosity will be

used:

$$Du_i^n = D^2u_i^n + D^4u_i^n \quad (15)$$

where

$$D^2u_i^n = \tilde{\epsilon}_2 \Delta x^2 u_{xx} \approx \tilde{\epsilon}_2 \Delta x^2 (u_{i-1}^n - 2u_i^n + u_{i+1}^n) \quad (16)$$

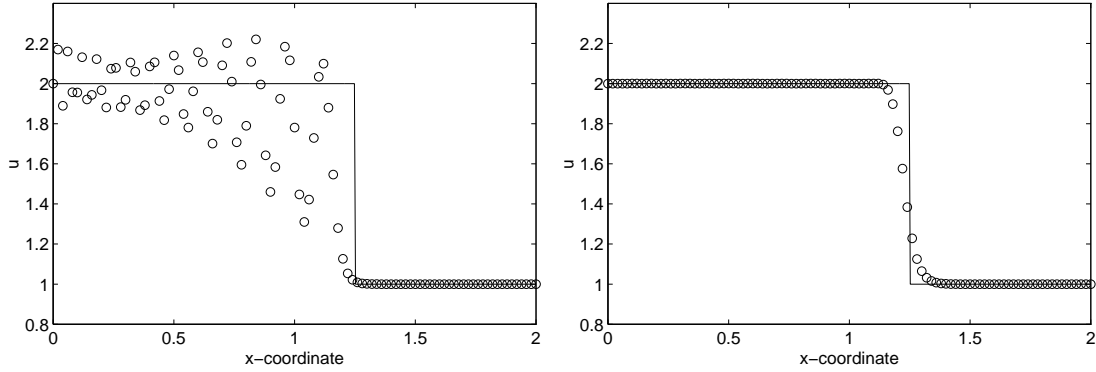
$$D^4u_i^n = \tilde{\epsilon}_4 \Delta x^4 u_{xxxx} \approx \tilde{\epsilon}_4 \Delta x^4 (u_{i-2}^n - 4u_{i-1}^n + 6u_i^n - 4u_{i+1}^n + u_{i+2}^n) \quad (17)$$

Because the original 3D problem is non-linear, it is necessary to extend the concept of dumping of numerical oscillations to the nonlinear equations. In this case some non-linear generalization of the artificial viscosity of second order will be used.

$$D^2u_i^n = \tilde{\epsilon}_2 \Delta x^3 \frac{\partial}{\partial x} |u_x| u_x = \tilde{\epsilon}_2 \Delta x^2 (\epsilon_{i+1/2} u_x - \epsilon_{i-1/2} u_x) \quad (18)$$

$$\epsilon_{i+1/2} = \begin{cases} |u_{i+1} - u_i| & \text{for } |u_{i+1} - u_i| < \epsilon_{lim} \\ \epsilon_{lim} & \text{for } |u_{i+1} - u_i| \geq \epsilon_{lim} \end{cases}$$

The ϵ_{lim} is an adjustable parameter which determines the amount of viscosity added into the scheme. It is easy to see that this non-linear artificial viscosity behaves like the linear one in the regions where the solution is strongly oscillating and just in the smooth parts its effect is different. Also here the Riemann test case was used, but this time the non-linear Burger's equation $u_t + uu_x = 0$ was solved. The significant improvement of the solution is obvious from the figure 2.



(a) without artificial viscosity

(b) with artificial viscosity

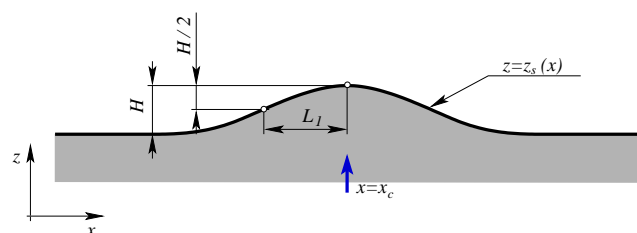
Figure 2: The 1D non-linear test of Wendroff scheme

The coefficients $\tilde{\epsilon}_2, \tilde{\epsilon}_4 \in \mathbb{R}$ are constants. However, since the added dissipation terms modify the original PDE the dissipation coefficients should be kept as small as possible.

7 Application

7.1 Wind-tunnel scale numerical experiments

Flow over low, smooth hills in 2D and 3D. The main impulse for the computations presented further in this section was the paper *Kim et al.* [12]. Following the experimental setup presented there, we have performed a series of computations of flow field and dispersion in 2D. This was further extended for similar, but 3D geometry. According to data published in *Kim et al.* [12] we have chosen 2D domain with four different sinusoidal single-hill terrain profiles having the following parameters:



Hill	slope	height H	length L_1
S3H4	0.3	4 cm	6.67 cm
S3H7	0.3	7 cm	11.67 cm
S5H4	0.5	4 cm	4.0 cm
S5H7	0.5	7 cm	7.0 cm

Figure 3: Hill geometry for 2D problems

Table 3: 2D hill setup

The notation we use here to distinguish between hills with different slopes and heights is the same as in *Kim et al.* [12]. It means the $SxHy$ stands for the hill with maximum slope $0.x$ and height y cm.

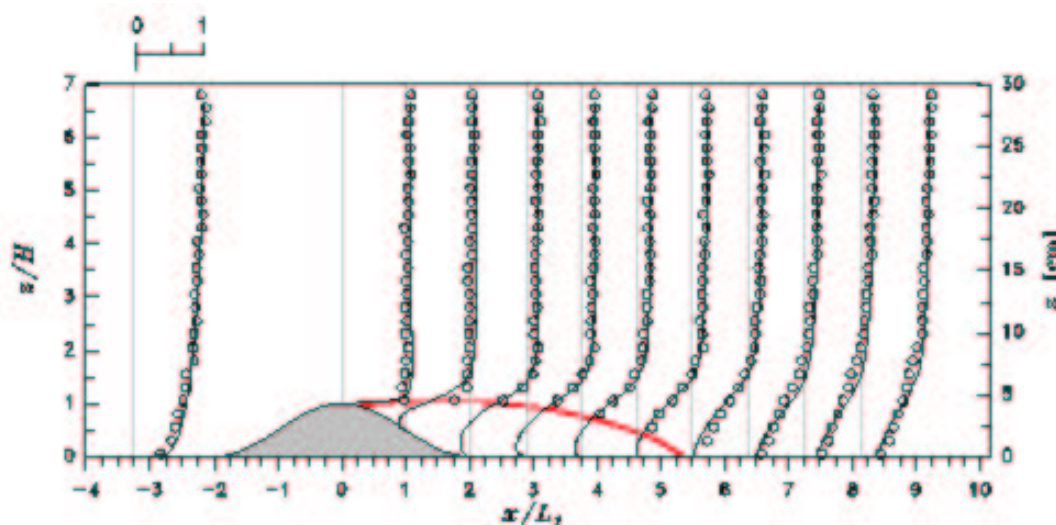


Figure 4: Vertical profiles of mean velocity U/U_∞ over the single hill $S5H4$ (\circ , experiment; $-$, low- Re -number model) Reprinted from *Kim et al.* [12]

In the above results we see the massive separation on the lee-side of the hill. Similar was observed in *Almeida, Durão, & Heitor* [1] and *Ferreira, Silva, Viegas, & Lopes* [10], *Ferreira et al.* [9]. The results that we have obtained for this case are shown in the following figures.

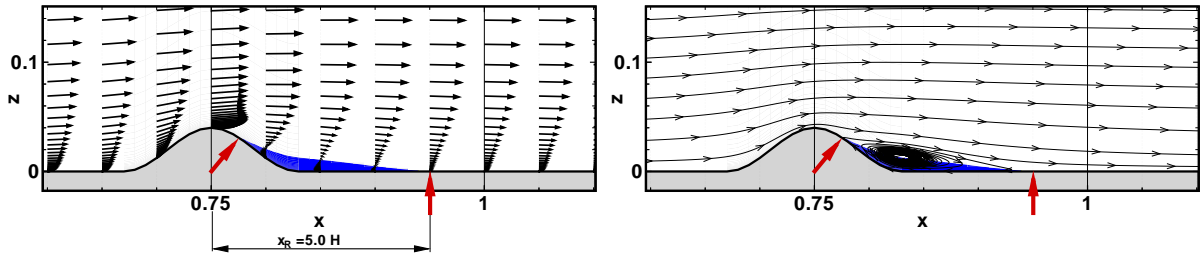


Figure 5: Flow over S5H4 hill. Separation and reattachment points marked by arrows.

Our results show relatively good agreement with observation in the case of separated flow over S5 hills. The shape of recirculation zone we have obtained, slightly differs from that observed or computed by another method as it is shown in figure 4. However the match between experimental results and our predictions can be judged as excellent when taking into account the simplicity of the algebraic turbulence model we have used.

So as in 2D case also here we can find a recirculation zone at the downwind side of the hill. The flow structure in this region is quite complicated and is difficult to visualize. In the following figure 6 the detail of surface wind direction vectors is drawn together with the color contours of negative part of longitudinal velocity u .

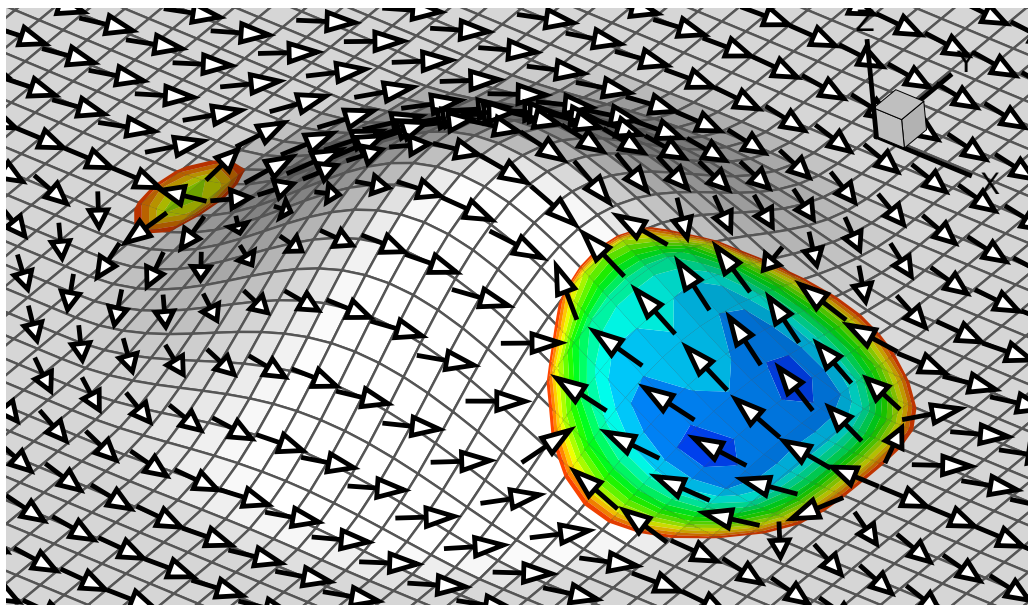


Figure 6: Surface wind direction & negative longitudinal velocity contours (in recirculation zone)

In the above figure we can also observe the stagnation point at the upwind hill foot. Almost the same vortical separation behind axially symmetric hill was observed in *Simpson, Long, & Byun* [16], where the following figure was published:

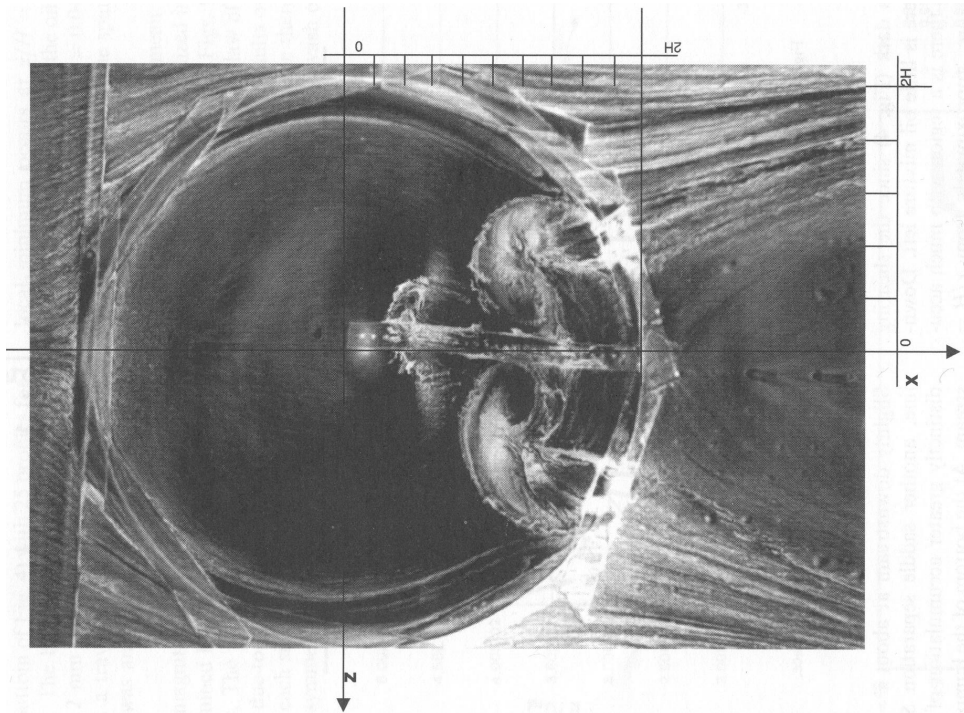


Figure 7: Surface wind patterns behind 3D hill *Reprinted from Simpson et al. [16]*

The main part of pollution dispersion modelling tests we have performed, was made for two-dimensional S5H4 hill. The flow is separated in this case and that is why the classical Gaussian plume models will fail here. We have assumed a continuous point sources placed at different heights at upwind and downwind base of the hill. The setup is clear from the following figure 8, where for clarity also the recirculation cavity region is drawn according to our computation.

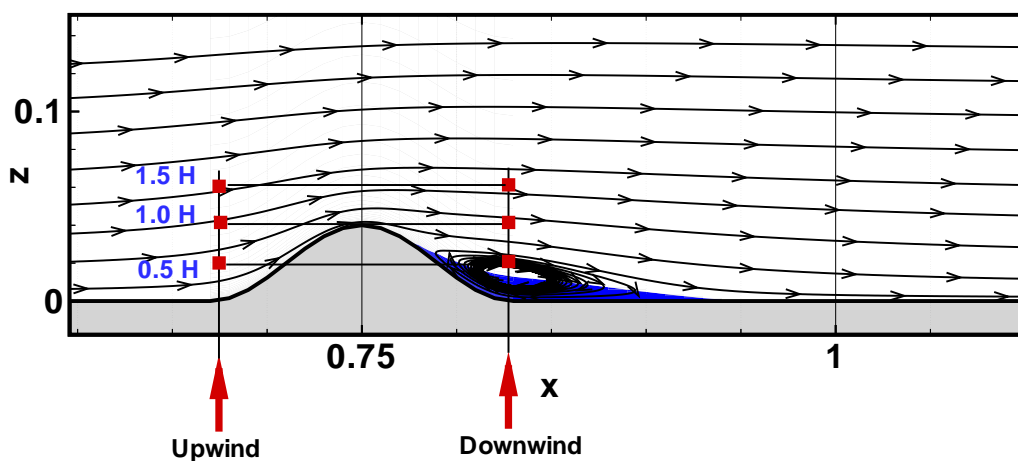


Figure 8: Point source positions in the vicinity of 2D S5H4 hill

The choice of the point-source positions was made in order to show the influence of hill itself so as the effect of recirculation on the large scale mixing.

Some experimental results confirming at least qualitatively the character of our results can be found in studies *Arya et al. [2]* and *Gong [11]*. A very similar numerical and experimental results were published in *Castro & Apsley [7]*.

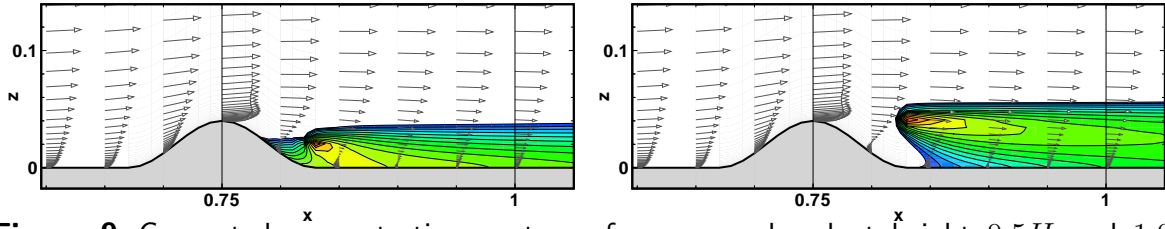


Figure 9: Computed concentration contours for source placed at height $0.5H$ and $1.0H$ downwind from the hill.

Almost the same numerical results were obtained in *Castro & Apsley* [7] as can be seen in the following figures reprinted from this paper.

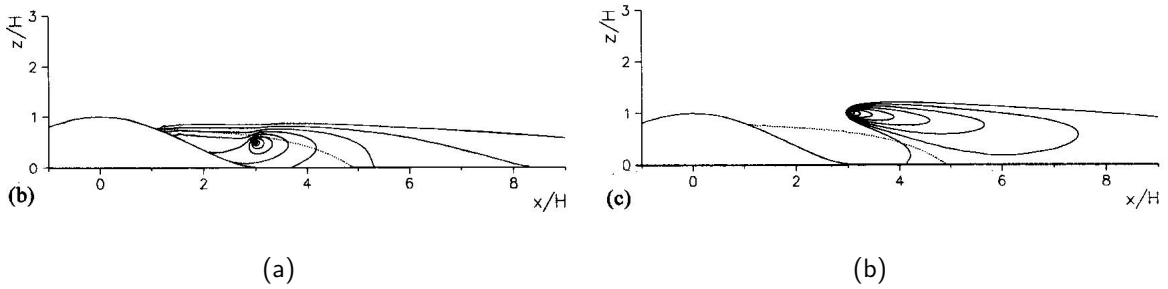


Figure 10: Computed contours of $\chi = CUH^2/Q$ for releases over the base of sinusoidal hill . Source heights: (a) $0.5H$; (b) $1.0H$. (—) denotes the mean separation streamline. *Reprinted from Castro & Apsley* [7]

7.2 Real scale numerical experiments

In this section we would like to present some first real terrain computations and results. The numerical implementation of our model to the real complex terrain flows will be shown in a little bit more detail. Two basic situations will be discussed. The first, and basic one, with steady boundary conditions and the second with unsteady boundary condition setup.

In the steady case we will describe the computational setup in detail including the specific treatment of boundary conditions and computational domain which are quite different from the wind-tunnel scale simulations presented in the previous chapter.

In the second test case we will go a little bit closer to the reality. We wish to try whether it would be possible to use our numerical model to solve problems where the boundary conditions vary in time. The problem we tried to solve is the simulation of 24 hours period with the time-dependent forcing based on measured wind field.

The model domain covers the area of the Mediterranean coast from Spain up to Italy. More precisely the domain lies between 2 and 8 degrees of longitude and 41 and 45 degrees of latitude. This domain including the terrain profile is shown in the following figure.

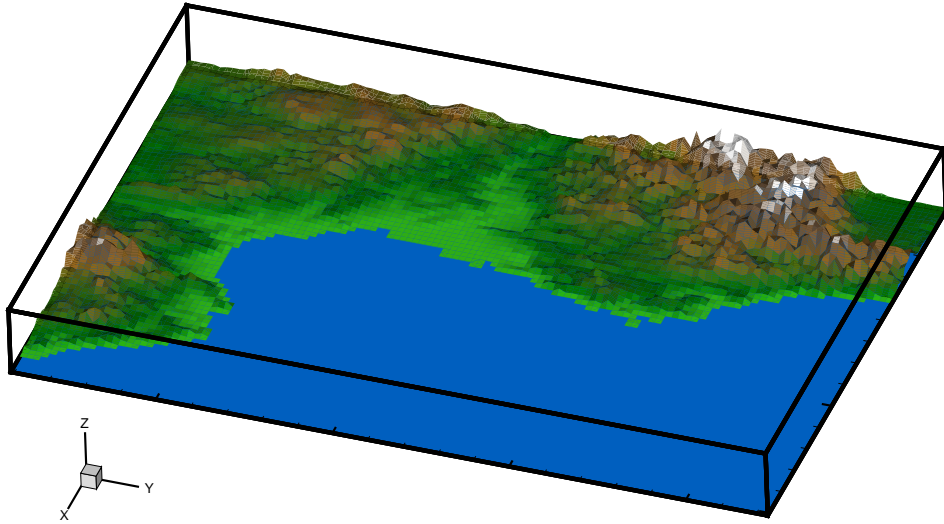


Figure 11: 3D domain with real terrain topography

The dimensions of this region are approximately 487×444 km with maximum terrain elevation 3406 m.

The topography data with resolution 30 angular seconds can be obtained from the United States National Geophysical Data Center (NGDC) from the resources of National Oceanic and Atmospheric Administration (NOAA).

Using this data we construct an initial grid with $120 \times 80 \times 40$ cells with horizontal resolution 3 angular minutes. The vertical dimension of computational domain was chosen to be 5 km which seems to be optimal even for the region of Alpes where the terrain elevation is quite high. The resulting velocity field computed using constant velocity prescribed at the top of the domain is shown in the following figure:

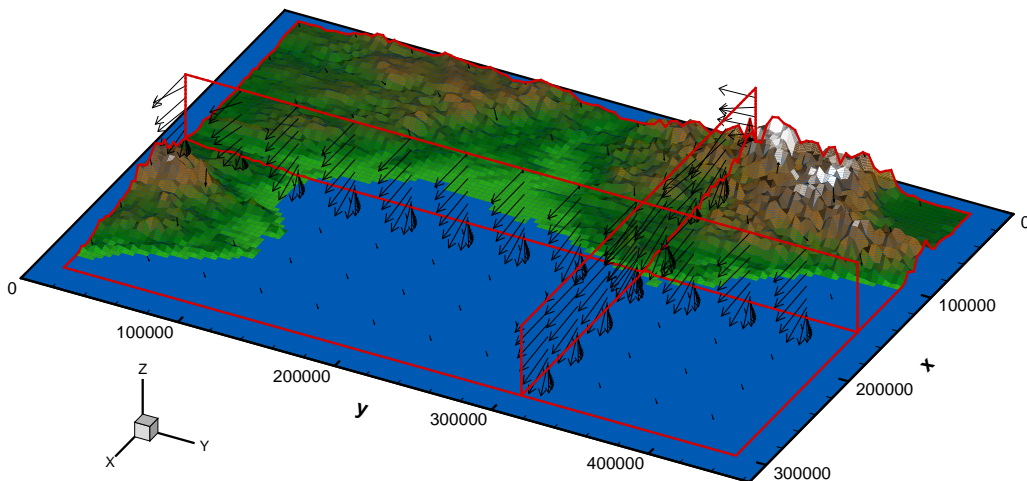


Figure 12: Wind velocity vectors, constant velocity at the upper boundary

In the above figure 12 the velocity vectors are drawn in two cutplanes with cross-section located close to Toulon. The near ground wind vectors are also indicated.

A better idea about the real boundary data we can get from the following figure where the contours of total velocity and wind direction vectors.

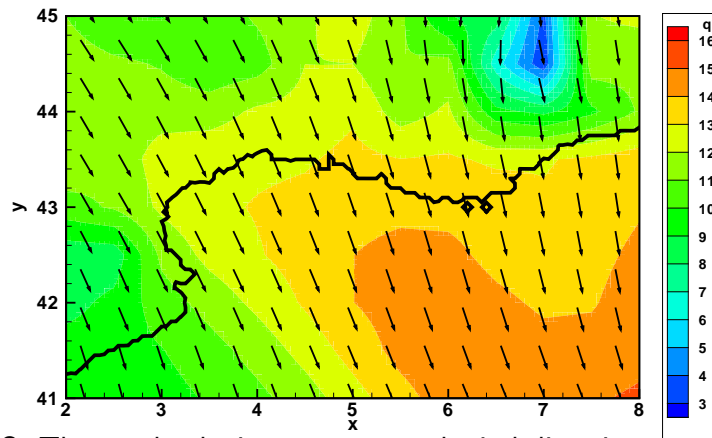
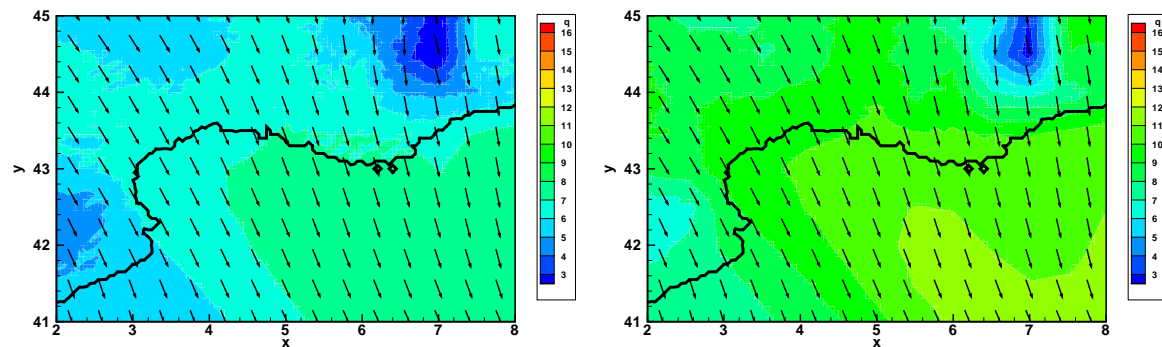


Figure 13: The total velocity contours and wind direction vectors at 5000m

The results obtained using the above mentioned setup are presented in the following section.

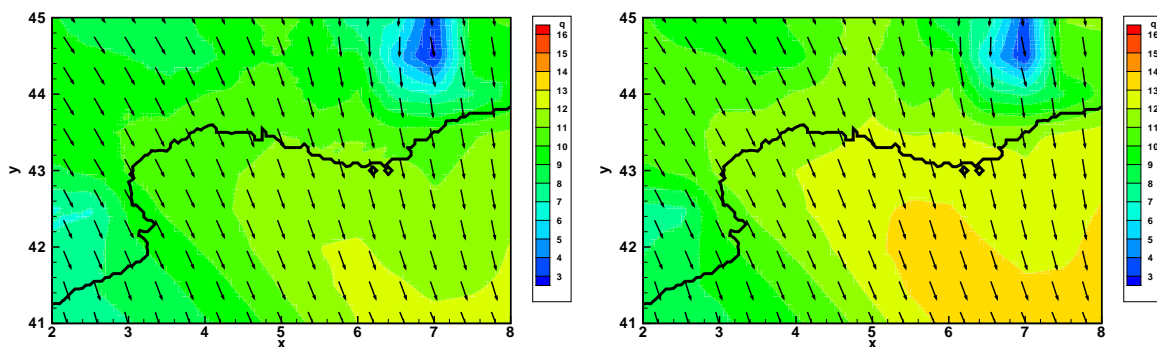
7.3 Numerical results

The results for the above specified test case are presented in the form of contours of total velocity and wind direction vectors at different heights above terrain.



(a) 110m

(b) 750m



(c) 1440m

(d) 3000m

Figure 14: The total velocity contours and wind direction vectors

More interesting problem appears in the case of real time-dependent boundary data prescription. The global character of the results obtained for this case seems to agree with our expectations. The velocity magnitude decays when approaching the ground. The originally smooth (large-scale purely) velocity field prescribed at the upper boundary is becoming perturbed by topography at the horizontal scales corresponding to the orography-grid resolution in the proximity of earth's surface.

The complexity of the problem will be more clear from the following figures 15 and 16, where profiles are drawn as line graphs periodically every 6 hours.

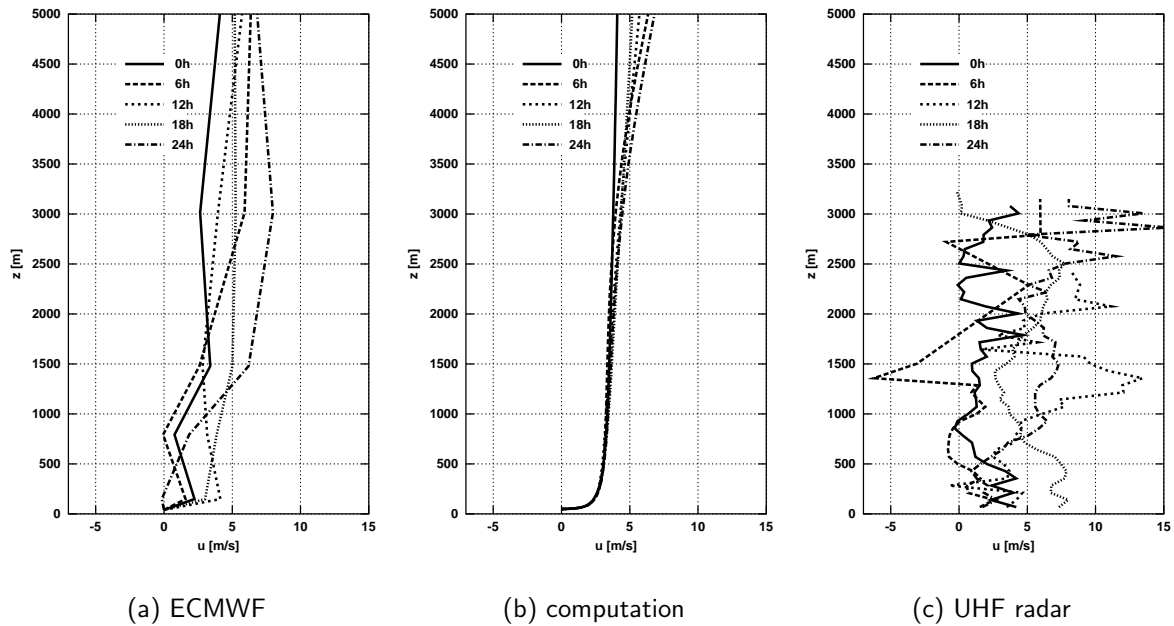


Figure 15: Comparison of u -component profiles for 21. June 2001 at Saint Chamas

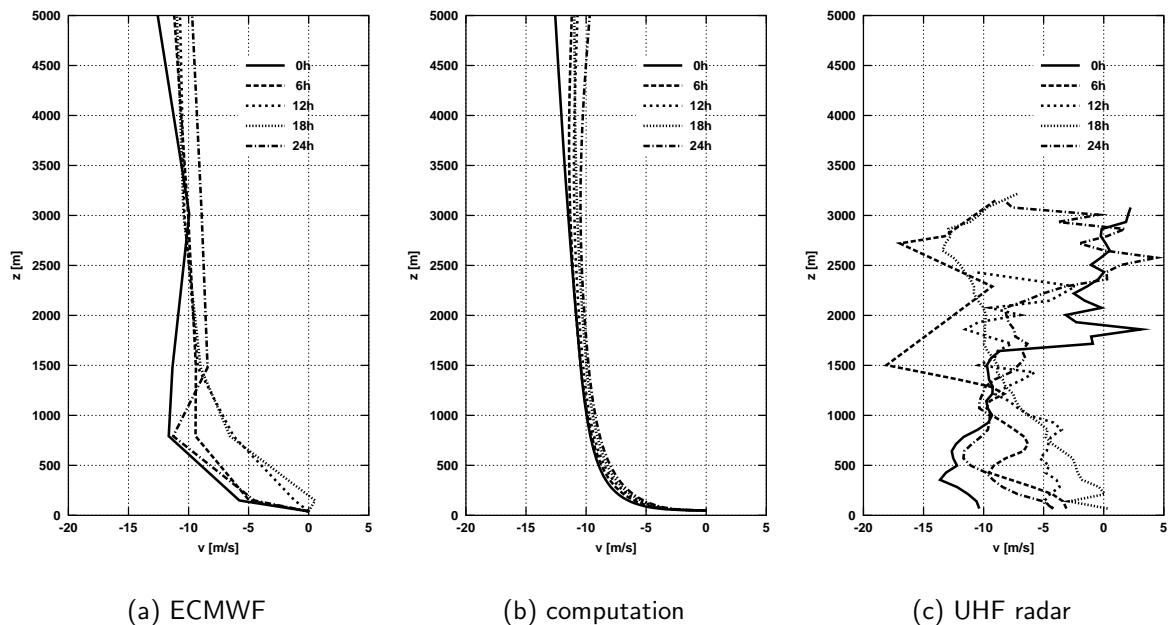


Figure 16: Comparison of v -component profiles for 21. June 2001 at Saint Chamas

From the above figures is clear that the complexity of wind-profiler data are not fully reproduced neither by ECMWF nor with our model. Even if some general tendency is the same for our results and ECMWF data we have to take a closer look where are the main differences and what are the possible causes. In the following set of figures we may observe the differences in detail.

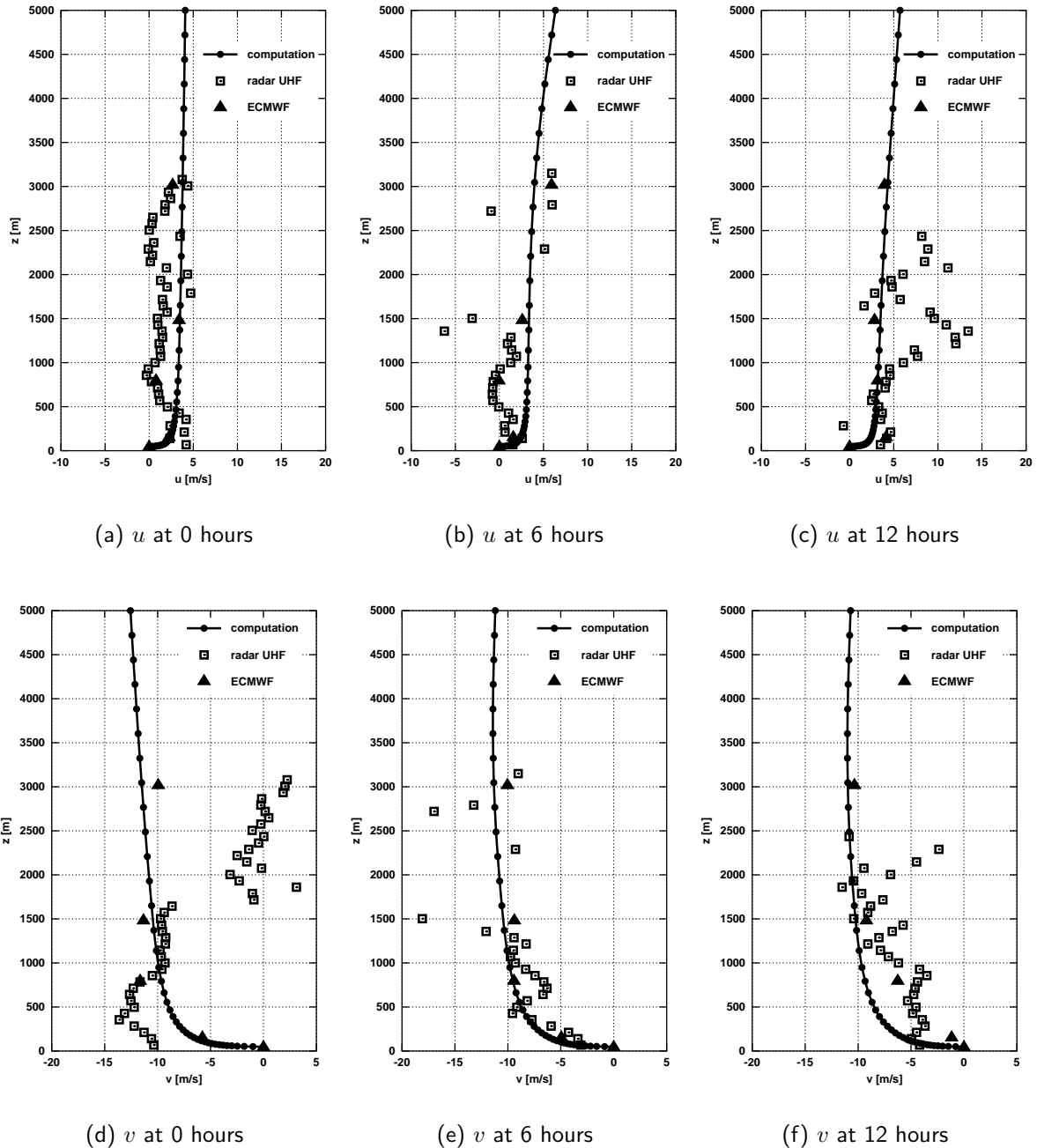


Figure 17: Comparison of u - and v - component profiles for 21. June 2001 at Saint Chamas

Taking a closer look to the above figures the comparison of our results with the others (especially with the ECMWF data) don't looks so disappointing at all. In many cases we are very close to either ECMWF or wind-profiler data. However there are still some important differences in the results and it is possible to see some general tendencies in these differences.

8 Conclusions & Perspectives

Throughout of this work, a significant effort has been made to provide balance between mathematical formulation, numerical solution and physical interpretation of the problem. That is why it may be difficult to draw any simple and consistent conclusion to the whole work. Thus we start at this place with summarizing the achievements of each part separately and checking up whether the main objectives of the work were achieved.

- I. In the first part of the work we have formulated mathematically the basic governing principles of the atmospheric flows. A special effort has been made to understand and interpret the meaning of these governing equations and separate terms involved in them. This helped us to fulfill the main objective of the physical part of the work, i.e. to chose the optimal mathematical model for ABL modelling. According to scale analysis of the “full” system of governing equations of the atmospheric flows we have proposed and derived the three basic governing systems applicable to the ABL flows problems. These are the following:
 - (a) Reynolds averaged Navier-Stokes equations
 - (b) Boussinesq approximation
 - (c) ABL approximation

In this way, the main objective of the first part was completely fulfilled. In addition to the formulation of simplified models, we have also found and discussed the limits of applicability of each model. These limits clearly follow from the assumptions used to simplify the general governing system. Finally we have analyzed and discussed in detail some problems connected with variable density flows modelling. This, together with detailed discussion of turbulence modelling, will be a starting point for future continuation of our work in this field.

- II. The second, mathematical, part of the work introduces the numerical methods used to solve the above mentioned mathematical models of atmospheric flows. For each of these models suitable numerical schemes were proposed and described in the detail. Special chapter was devoted to detailed study of one of these schemes. This analysis has helped us to understand correctly the influence of numerical method on the behavior of the resulting solution. The methodology used to analyze the properties of the scheme has general validity and can be applied also to the other numerical methods. In short, we have shown the different numerical techniques applicable to ABL modelling and presented some of the basic tools that may help us to analyze and understand the properties of numerical method. So we have reached the main goal of this part⁷. As in the first part, also the mathematical part contains some additional material that can be used for future work in the area of ABL modelling. Two basic ways of possible future improvement of ABL models were discussed. Firstly some alternative methods for pressure resolution in incompressible models were presented. The second topic that should be addressed in the future models is the possible use of compressible models. Some of the links between these two problems were pointed out.
- III. In the last main part of the work we have concentrated on two basic topics, i.e. the validation and application of our mathematical and numerical model. In the “validational”

⁷Formulated in the Introduction

part we have applied our model to the wind-tunnel scale problems in 2D and 3D including the flow-field and pollution dispersion computations. During number of numerical tests the method has proved good agreement with numerous experimental measurements and reference computations in both flow and pollution resolution in 2D and 3D. The modification and adjustment of turbulence model for small-scale flows has been successfully tested. Throughout of these validation testing the numerical method has shown its robustness, efficiency and accuracy in the range of tests we have performed. It means we have satisfied the main objectives that have been formulated for this part of the work. In the rest of the part we have demonstrated the applicability of our model for real terrain, large scale simulations including the use of some meteorological inputs in problem setup. In these realistic simulations we have successfully applied the modified boundary conditions, used the orography databasis and meteorological data sources. We were able to initialize the model with the minimum necessary information, to get in relatively short time the valuable detailed results concerning the flow field structure at the local scale.

From the above overview follows, that all the objectives and goals of the work were fulfilled. We have presented all the material necessary to develop, understand and use the actual working models of ABL flows including the pollution dispersion simulations. In addition to this complete summary of the actual stage of our research, we have presented and discussed some of possible ways leading to the extension of the current model and to the creation of the new generation of atmospheric model. Let's finally summarize in short some of the topics of possible improvements, continuation and discussion:

- Application of the actual model, i.e. the Boussinesq approximation, to the weakly stratified flows. The model is ready for this kind of simulation. Some additional modifications will be necessary in initial and boundary condition setup for potential temperature.
- Modify the actual method for the computation of unsteady problem. It can be basically done in two ways. The first one introduces the sub-iterations in artificial time to the presented model. This is the easiest way how to modify our existing model with artificial compressibility assumption, however the open question is the optimality of this approach with respect to the required computational cost. The second way to develop the time-dependent method is to apply some other pressure resolution technique, as it has been discussed in the work. However this requires larger changes in the actual code.
- Implement some more sophisticated model of turbulence that will be able to treat correctly the complex terrain flows under stronger stratification. In such situations the buoyancy effects can have significant impact on the flow structure. Another point that should be addressed when searching for future turbulence model, is its ability to resolve the turbulence at urban scale problems.
- Develop a new generation model, that will be able to treat naturally the variable density, unsteady, highly turbulent flows. This can be e.g. done by employing the full "compressible"⁸ model, solved by some implicit (because of the necessity of large time steps to perform simulations at long time-scales) method equipped by suitable preconditioning (because of the low-Mach, high-Reynolds number flows). This model can use with advantage some of the recent, specialized LES models.

⁸In the sense of variable density model.

- Improve the physical description of some parameters. It means e.g. implement and improve the parametrization of heat and moisture fluxes, surface properties parametrization for sea- and land-scape. Test the model for non-uniform surface roughness including the wind driven changes in sea surface roughness and flow over urban areas. In the field of pollution dispersion it is possible to extend the use of the actual model by implementing the particle (e.g. dust) transport model including the release and deposition of contaminant, or include some basic chemistry model to treat also some non-passive pollutant dispersion.

At the end of the work, let's just remind, that not all of our experience and results was possible to involve in this work and some additional information can be found in section 8 and references therein.

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Published works

- [[1]] Bodnár, T. - Kozel, K. - Sládek, I.: Matematické modelování a numerické řešení proudění v mezní vrstvě atmosféry (in Czech) *Mathematical Modelling and Numerical Solution of Atmospheric Boundary Layer Flows* In: Topical Problems of Fluid Mechanics 96. Prague : Academy of Sciences of the Czech Republic, Institute of Thermomechanics, 1996, s. 3-4. ISBN 80-85918-17-X.
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