Abschlussbericht:

Entwicklung und Evaluierung eines meteorologischen Modellsystems zur Folgenabschätzung von Umwelteingriffen auf Klima und Luftqualität

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Zielsetzung und Anlass des Vorhabens

Entwicklung eines meteorologischen Programmsystems (**METRAS$^+$**) zur Beurteilung der Wirkung von Umwelteingriffen auf klimatische und lufthygienische Parameter. Ziel ist die Bereitstellung eines kostengünstigen Planungsinstrumentes für Behörden und Beratungsunternehmen, das geplante nationale Qualitätsnormen (VDI-Richtlinie) erfüllt. Vergleichbare Modelle existieren bislang nur im wissenschaftlichen Bereich, sind kaum qualitätsgesichert und werden u.a. aus wirtschaftlichen Erwägungen nur in Ausnahmefällen eingesetzt.

Darstellung der Arbeitsschritte und der angewandten Methoden

Das Programmsystem **METRAS$^+$** setzt sich aus den vier Programmkomponenten THD, GRITOP, METRAS PC und EVA zusammen, die der Vorbereitung, Durchführung und Qualitätssicherung mesoskaliger Modellrechnungen dienen. Alle Programmkomponenten laufen unter einer gemeinsamen, anwenderfreundlichen Windowsoberfläche.
Die Komponenten THD (Aufbereitung eines gesamtdeutschen Topographiekatasters) und EVA (Qualitätssicherung mesoskaliger Modellrechnungen nach der geplanten VDI Richtlinie 3783, Blatt 7) wurden neu entwickelt, die Komponenten GRITOP (Erzeugung von METRAS PC Modellgittern aus Topographierohdaten) und METRAS PC (mesoskaliges Transport- und Strömungsmodell) - aufbauend auf Vorläuferversionen - weiterentwickelt und in ihrer Funktionalität erheblich erweitert. Die Programmierung aller Programmkomponenten erfolgte in FORTRAN 90/95. Die Windowsoberfläche von **METRAS$^+$** verwendet als Schnittstellen zu den API-Routinen der Windows-Betriebssysteme die WINTERACTER-Bibliotheken (Interacter Software Services Ltd.). Die Kommunikation zwischen **METRAS$^+$** und den vier Programmkomponenten setzt auf einem „Shared Buffer"-Prinzip auf, bei dem Daten zwischen den verschiedenen Applikationen über reservierte Arbeitsspeicherbereiche des Betriebssystems ausgetauscht werden. Alle Programme wurden umfangreichen Testrechnungen unterzogen.
Zur Evaluierung gemäß VDI-Richtlinie wurden zwei Messdatensätze beschafft, geprüft und aufbereitet.
Zusätzlich zu einem Programmhandbuch für das Gesamtsystem wurde für jede Programmkomponente eine Dokumentation (englisch/deutsch) erstellt.

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Ergebnisse und Diskussion

Die Entwicklung des Programmsystems **METRAS⁺** und die Testrechnungen konnten soweit abgeschlossen werden, dass in Kürze eine Betaversion freigegeben werden kann:
Die Windowsoberfläche ist programmiert und einer Vielzahl von Testrechnungen unterzogen worden. **METRAS⁺** ist unter den Betriebssystemen Windows 98 / NT / 2000 Professional voll funktionsfähig. Insbesondere kommunizieren alle Programmkomponenten untereinander stabil und fehlerfrei.
Alle vier Programmkomponenten wurden vollständig programmiert und umfangreichen Testrechnungen unterzogen.
Die Komponente THD konvertiert fehlerfrei Daten des gesamtdeutschen Topographiekatasters, was anhand mehrerer Gebietsausschnitte sowohl für die alten und neuen Bundesländer als auch gebietsübergreifend überprüft wurde.
Die Komponente GRITOP wurde anhand von Modellgebieten für verschiedene Regionen Europas sowie für unterschiedliche Datenformate und Projektionssysteme getestet. In allen Fällen wurden die Rohdaten (auch in der Kombination unterschiedlicher Formate und Systeme) korrekt in METRAS PC Modellgitter umgerechnet.
In die neue Version des mesoskaligen Modells METRAS PC wurden u.a. eine neue Turbulenzschließung, ein verbessertes Initialisierungsverfahren, wolkenmikrophysikalische Prozesse, Stofftransportprozesse und das Blendhöhenverfahren zur Berechnung bodennaher Flüsse aus der wissenschaftlichen Modellversion eingebaut. Die neue Modellversion wurde anhand der vorgesehenen VDI-Evaluierungsfälle und weiterer Modelltests geprüft. Dabei wurden in zwei Testfällen noch Unterschiede zu der bereits evaluierten wissenschaftlichen Modellversion festgestellt, deren Ursache noch kurz vor Projektende festgestellt und beseitigt werden konnte. Die Betaversion von **METRAS⁺**, deren Freigabe für Ende 2001 geplant ist, wird diese korrigierte und evaluierte Version von METRAS PC enthalten. Auch die Komponente EVA wurde erfolgreich daraufhin getestet, dass die Kriterien der VDI-RL richtig abgefragt und bewertet, die METRAS PC Ergebnisse eingelesen und konvertiert und das Evaluierungszertifikat den Qualitätskriterien gemäß erstellt wird.
Für das gesamte Programmsystem wurden umfangreiche Programmdokumentationen sowie ein Handbuch in jeweils englischer und deutscher Version erstellt.

Öffentlichkeitsarbeit und Präsentation

Das Programmsystem **METRAS⁺** wurde auf der Deutsch-Österreichisch-Schweizerischen Meteorologen-Tagung vom 18.-21.9.2001 in Wien im Rahmen eines Vortrages erstmals der Öffentlichkeit vorgestellt. Die schriftliche Vortragsversion wurde in den Tagungsbeiträgen veröffentlicht. Schon im Vorfeld der Tagung gingen aufgrund der Vortragsankündigung Nachfragen zu **METRAS⁺** ein, die auf ein hohes Interesse an dem Produkt schließen lassen.
Während der Projektlaufzeit wurden Informationen zu dem Projekt im Internet unter der Adresse http://www.metcon-umb.de/Uber_uns/METRAS_/metras_htm der Öffentlichkeit zugänglich gemacht. Auf die ebenfalls im Internet angekündigte Freigabe einer Betaversion von **METRAS⁺** gingen innerhalb kurzer Zeit mehrere Vorbestellungen ein. Dies zeigt ebenfalls deutlich, dass mit den Ergebnissen des Projekts eine auf dem Gutachten- und Beratungssektor im Bereich von Regionalklima und Lufthygiene bestehende Lücke geschlossen wird.
Um die breite Anwendung qualifizierter Untersuchungsmethoden im Umweltconsulting zu fördern, ist geplant, **METRAS⁺** nicht kommerziell zu vertreiben und das Programmsystem interessierten Anwendern gegen einen geringen Kostenbeitrag zur Verfügung zu stellen. Vertrieb und Öffentlichkeitsarbeit (z.B. Bereitstellung aktueller Informationen im Internet) sollen vom Meteorologischen Institut der Universität Hamburg geleistet werden.

Fazit

Das neu erstellte Programmpaket **METRAS⁺** wird mit Sicherheit in Beratungsunternehmen und Behörden vielfältige Einsatzmöglichkeiten finden, zumal es zu geringen Kosten zur Verfügung steht. Die Vorstellung des Programmsystems bei der Meteorologentagung in Wien hat vielseitiges Interesse ausgelöst. Dieses galt nicht nur für das gesamte Programmsystem, sondern auch für Teilkomponenten. Insbesondere galt das Interesse neben METRAS PC den Programmen GRITOP und EVA. Auch Entwickler anderer mesoskaliger Modelle waren hieran interessiert, um ihr Programm einer METRAS PC vergleichbaren Qualitätssicherung zu unterziehen. Ein wichtiges Ziel dieses Projektes, die vorhandenen Modelle für Umweltuntersuchungen zu einem höheren Standard zu führen, scheint damit erreicht.

Verzeichnis der Anhänge

Band 1:

1. Handbuch zum Programmsystem **METRAS$^+$** (deutsche Version)
2. Dokumentation der **METRAS$^+$**-Programmkomponente THD (deutsche Version)
3. Dokumentation der **METRAS$^+$**-Programmkomponente THD (englische Version)
4. Dokumentation der **METRAS$^+$**-Programmkomponente GRITOP (deutsche Version)
5. Dokumentation der **METRAS$^+$**-Programmkomponente GRITOP (englische Version)

Band 2:

6. Dokumentation der **METRAS$^+$**-Programmkomponente METRAS PC (englisch)
7. Dokumentation der **METRAS$^+$**-Programmkomponente EVA (deutsche Version)
8. Dokumentation der **METRAS$^+$**-Programmkomponente EVA (englische Version)
9. Tagungsbeitrag zur Deutsch-Österreichisch-Schweizerischen Meteorologen-Tagung DACH 2001, 18. bis 21. September 2001, Wien
10. CD: Programmsystem **METRAS$^+$** mit Installationsroutinen, Onlinehilfen und Programmdokumentationen (vorläufige, unveröffentlichte Programmversion)

Documentation of the Mesoscale Transport and Fluid Model 'METRAS PC' as part of model system 'METRAS+'

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Chapter 1

Introduction

The model METRAS PC (release 2.0) is based on the **ME**soscale **TRA**nsport and fluid (**S**tream) Model METRAS (September 2001; Schlünzen, 1988, 1990). The documentation uses an earlies description of model METRAS by Schlünzen et al. (1996). METRAS PC is based on the primitive equations, ensuring the conservation of mass, momentum and energy. The equations are solved three–dimensional in a terrain—following coordinate system. Only few approximations are applied, which ensure a wide range of model applications. The simplifications used are the anelastic assumption as well as the Boussinesq approximation. Additionally, a constant Coriolis parameter is used in the model area. The use of a non–uniform grid allowes a high resolution in interesting model areas. Wind, temperature, humidity, cloud– and rain–water–content as well as concentrations are derived from prognostic equations, whereas density and pressure are calculated from diagnostic equations.

Subgrid scale turbulent fluxes are parameterized by first order closure theory, using different formulations for the exchange coefficients (Lüpkes and Schlünzen, 1996). For the calculation of surface fluxes a blending hight concept can be applied (von Salzen et al., 1996) or mean parameters are calculated. Both schemes allow to take into account subgrid–scale surface characteristics. The roughness length z_o over water depends on the wind velocity using Charnock's formula. A Kessler–type cloud microphysics parametrization scheme is applied when simulating clouds and rain. The radiation balance in the atmosphere is calculated by a two–stream approximation that takes into account transmission and refraction by water vapour and hydrometeors. Pollutant dispersion is calculated with inclusion of dry deposition processes. In summary, METRAS PC fulfills all demands on an 'up–to–date' mesoscale model.

The mother model METRAS applied in research has some additional features: some more additional exchange coefficients can be selected, the model may be nested in larger scale values and chemical reactions are considered. These features need, however, still to be further tested in the frame of research work before they should be transfered to a PC version.

In Chapter 2 and 3 of this model description the equations, approximations and parameterizations used in METRAS PC, are described. In Chapter 4 the discretization and the numerical schemes and in Chapter 5 the boundary conditions used in the model are presented. In Chapter 6 the initialization of the model is described. Chapter 7 gives an overview on the validation of METRAS PC. The implemented parameter values of surface characteristics and deposition modelling are summarized in Appendix A.1 and A.3.

The current model description corresponds to the METRAS PC Fortran 90 version, release 2.x, dated October 2001.

Chapter 2

Derivation of Model Equations

This chapter contains a derivation of the basic equations and the used approximations.

2.1 Basic Equations

The basic prognostic equations of the model are given by the equation of motion (2.1), the continuity equation (2.2) and the conservation of heat, water and other materials (2.3). They are completed by the ideal gas law (2.4) and the definition of potential temperature (2.5) as diagnostic equations. The basic equations within a coordinate system rotating with the earth can be written (e.g. Dutton, 1976):

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho}\nabla p - 2[\Omega \times \mathbf{v}] - \nabla\Phi + \mathbf{F} \tag{2.1}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{2.2}$$

$$\frac{\partial \chi}{\partial t} + \mathbf{v} \cdot \nabla\chi = Q_\chi \tag{2.3}$$

$$v_i^k = \frac{R_i^k T}{p} \tag{2.4}$$

$$\theta = T\left(\frac{P_r}{p}\right)^{R/c_p}, P_r = 1000\ hPa \tag{2.5}$$

The three–dimensional velocity vector is described as $\mathbf{v}$, the gradient operator as ∇, density as ρ, pressure as p and time as t. Ω is the earth's angular velocity, Φ the geopotential and $\mathbf{F}$ are molecular forces, which are neglected within the model. χ stands for any scalar quantity including potential temperature θ, concentration C_j of a pollutant j or concentration of atmospheric water q_1^k, where $k = 1, 2, 3$ means vapour, liquid and solid phases.

Sources and sinks of a scalar quantity χ are described by Q_χ, e.g. the processes of condensation and evaporation for water vapour. The specific volume v_i^k stands for dry air ($i = 0$) and water ($i = 1$) in phase k and R_i^k or R for the individual or universal gas constant respectively. c_p is the specific heat at constant pressure and T the real temperature.

The equations above are not solved in the cartesian but in a terrain–following coordinate system. Thus the lower boundary conditions can be calculated easier for model applications over complex terrain.

2.2 Transformation to Terrain–following Coordinates

The transformation of the model equations from a cartesian system to a non–orthogonal coordinate system is described in (Schlünzen (1988) in detail. Within this coordinate system the vertical coordinate η is zero at the ground $z = z_s(x, y)$ and $\eta = z_t$ at the top of the model $z = z_t$:

$$\eta = z_t \frac{z - z_s(x, y)}{z_t - z_s(x, y)} \tag{2.6}$$

η–coordinates of this or a similar type are often used in mesoscale models (Pielke, 1984;

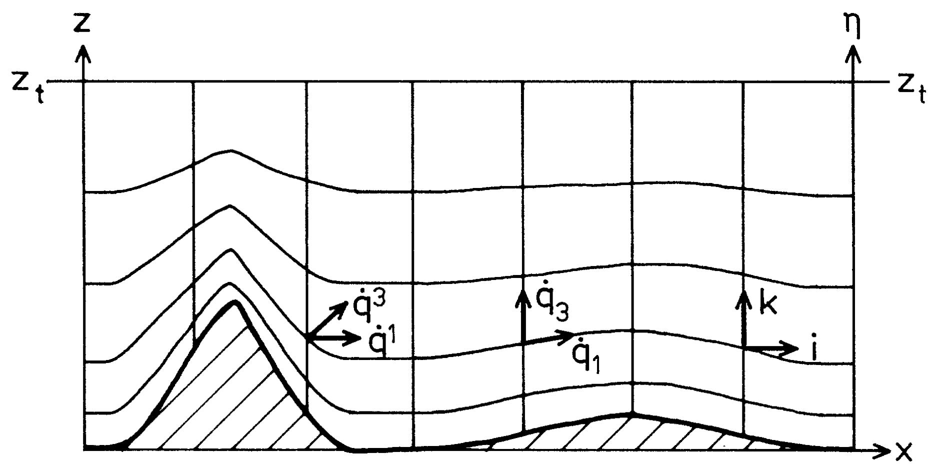

Figure 2.1: Schematic illustration of mountains, coordinate surfaces of η–coordinates, basis vectors **i**, **k** of a cartesian coordinate system X and $\dot{\mathbf{q}}_1$, $\dot{\mathbf{q}}_3$, $\dot{\mathbf{q}}^1$, $\dot{\mathbf{q}}^3$ of a terrain–following coordinate system.

Schlünzen and Schatzmann (1984)). Figure 2.1 schematically illustrates the location of coordinate surfaces η = constant for a horizontal uniform grid. Included are the basis vectors $\mathbf{i}, \mathbf{k}$ of a cartesian system X and the covariant ($\dot{\mathbf{q}}_\mathbf{i}$) and contravariant ($\dot{\mathbf{q}}^i$) basis vectors of a terrain–following system $\dot{X}$.

The model METRAS PC can be used for simulations of wind, temperature and concentration fields over areas of up to 800 x 800 km^2. Processes limited to relatively small areas (e.g. sea–land breezes) are not parameterized but solved explicitly by the model. In some cases it is necessary to resolve the interesting areas by a fine grid. However, even with today's computer resources it is impossible to obtain very high grid resolutions for the entire model area. In METRAS PC this problem is avoided by use of a horizontally non–uniform but orthogonal grid with minimum grid increments of about 20 m and maximum increments of about 5 km. The restrictions are caused by the numerics and parameterizations used (see below).

To reduce the number of grid–points, the coordinate system can be rotated against North in any desired angle (Niemeier, 1992). This rotation is taken into account when calculating the Coriolis force.

As mentioned above, the model equations are not only transformed to a terrain–following but also from a non–uniform to a uniform grid. Figure 2.2 schematically illustrates a possible grid structure for the area of the German Bight. The prognostic model equations (2.1)—(2.3) are transformed to the described coordinate system $\dot{X}$ (Schlünzen, 1988). The equations of momentum are given by

$$\begin{aligned}
\frac{\partial \rho \overset{*}{\alpha} u}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{u \frac{\partial \dot{x}^1}{\partial x} \rho \overset{*}{\alpha} u\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{v \frac{\partial \dot{x}^2}{\partial y} \rho \overset{*}{\alpha} u\right\} - \frac{\partial}{\partial \dot{x}^3}\left\{\dot{u}^3 \rho \overset{*}{\alpha} u\right\} \\
&\quad - \overset{*}{\alpha} \frac{\partial \dot{x}^1}{\partial x} \frac{\partial p}{\partial \dot{x}^1} - \overset{*}{\alpha} \frac{\partial \dot{x}^3}{\partial x} \frac{\partial p}{\partial \dot{x}^3} + f \rho \overset{*}{\alpha} v - f' d' \rho \overset{*}{\alpha} w
\end{aligned} \tag{2.7a}$$

$$\begin{aligned}
\frac{\partial \rho \overset{*}{\alpha} v}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{u \frac{\partial \dot{x}^1}{\partial x} \rho \overset{*}{\alpha} v\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{v \frac{\partial \dot{x}^2}{\partial y} \rho \overset{*}{\alpha} v\right\} - \frac{\partial}{\partial \dot{x}^3}\left\{\dot{u}^3 \rho \overset{*}{\alpha} v\right\} \\
&\quad - \overset{*}{\alpha} \frac{\partial \dot{x}^2}{\partial y} \frac{\partial p}{\partial \dot{x}^2} - \overset{*}{\alpha} \frac{\partial \dot{x}^3}{\partial y} \frac{\partial p}{\partial \dot{x}^3} - f \rho \overset{*}{\alpha} u + f' d \rho \overset{*}{\alpha} w
\end{aligned} \tag{2.7b}$$

$$\begin{aligned}
\frac{\partial \rho \overset{*}{\alpha} w}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{u \frac{\partial \dot{x}^1}{\partial x} \rho \overset{*}{\alpha} w\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{v \frac{\partial \dot{x}^2}{\partial y} \rho \overset{*}{\alpha} w\right\} - \frac{\partial}{\partial \dot{x}^3}\left\{\dot{u}^3 \rho \overset{*}{\alpha} w\right\} \\
&\quad - \overset{*}{\alpha} \frac{\partial \dot{x}^3}{\partial z} \frac{\partial p}{\partial \dot{x}^3} + f' \rho \overset{*}{\alpha} (u\, d' - v\, d) - \rho \overset{*}{\alpha} g
\end{aligned} \tag{2.7c}$$

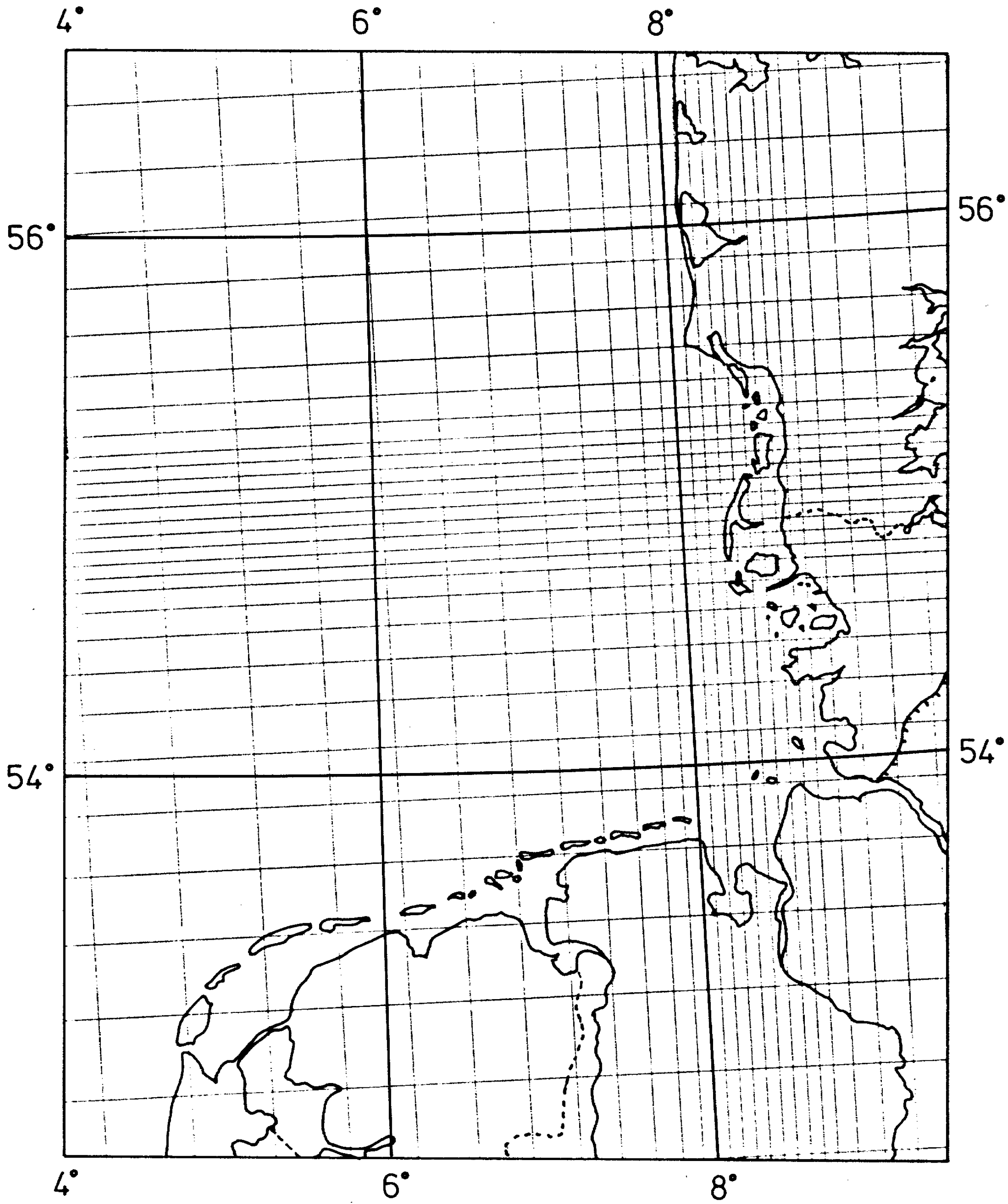

Figure 2.2: Schematic illustration of a cartesian grid focussing on the isle of Sylt.

The components of the wind vector **v** in cartesian coordinates are named u, v, w corresponding to the x–, y–, z–direction. The variables $d = \ sin\ \xi$ and $d' = \ cos\ \xi$ characterize the influence of a rotation of the coordinate system by an angle ξ against North. In the non–rotated case ($\xi = 0$) the components of the wind vector characterize the west–east, south–north and vertical winds. $\overset{*}{\alpha}$ denotes the grid volume. $\dot{x}^1$, $\dot{x}^2$, $\dot{x}^3$ and x, y, z are the coordinates of the used coordinate system $\dot{X}$ and the cartesian system X, respectively. The Coriolis parameters $f = 2\ \Omega\ sin\varphi$ and $f' = 2\ \Omega\ cos\varphi$ are calculated for the geographic latitude φ, and g is the acceleration of gravity.

The wind component $\dot{u}^3$ normal to the surface–boundary can be calculated from u, v, w by:

$$\dot{u}^3 \ = \ u\frac{\partial \dot{x}^3}{\partial x} + v\frac{\partial \dot{x}^3}{\partial y} + w\frac{\partial \dot{x}^3}{\partial z} \tag{2.8}$$

The transformed continuity equation is given by:

$$\frac{\partial \rho \overset{*}{\alpha}}{\partial t} + \frac{\partial}{\partial \dot{x}^1}\left\{\rho \overset{*}{\alpha}\, u\frac{\partial \dot{x}^1}{\partial x}\right\} + \frac{\partial}{\partial \dot{x}^2}\left\{\rho \overset{*}{\alpha}\, v\frac{\partial \dot{x}^2}{\partial y}\right\} + \frac{\partial}{\partial \dot{x}^3}\left\{\rho \overset{*}{\alpha}\, \dot{u}^3\right\} = 0 \tag{2.9}$$

The conservation of a scalar quantity χ can be written as:

$$\begin{aligned}\frac{\partial \rho \overset{*}{\alpha} \chi}{\partial t} \ &= \ -\frac{\partial}{\partial \dot{x}^1}\left\{u\frac{\partial \dot{x}^1}{\partial x}\rho \overset{*}{\alpha} \chi\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{v\frac{\partial \dot{x}^2}{\partial y}\rho \overset{*}{\alpha} \chi\right\} \\ &\quad -\frac{\partial}{\partial \dot{x}^3}\left\{(u\frac{\partial \dot{x}^3}{\partial x} + v\frac{\partial \dot{x}^3}{\partial y} + w\frac{\partial \dot{x}^3}{\partial z})\rho \overset{*}{\alpha} \chi\right\} - Q_\chi\end{aligned} \tag{2.10}$$

where Q_χ is the production term of χ.

2.3 Averaging the Basic Equations

The system of Equations (2.7)—(2.10) can be solved directly, as long as the spatial derivatives $\partial\psi/\partial\dot{x}^i$ of a variable ψ can be assumed as being constant over a spatial scale $\delta\dot{x}^i$ and a time scale δt. In the atmosphere this assumption is valid for spatial scales of about 1 cm and time scales of about 1 sec (Pielke, 1984). If one tries to solve the system (2.7)—(2.10) for typical mesoscale phenomena in a horizontal scale of about 100 km and a vertical extension of about 10 km, it would be necessary to calculate solutions at about 10^{20} grid points. Since this exceeds the capacity of existing computers, the equations have to be averaged, i.e. they have to be integrated in time and space.

Every dependent variable ψ is decomposed into an average $\overline{\psi}$ and a deviation ψ' from the average. $\overline{\psi}$ represents the average of ψ over the finite time increment Δt and a surrounding volume $\Delta x \cdot \Delta y \cdot \Delta z$ (see Pielke, 1984)::

$$\overline{\psi} := \int_t^{t+\Delta t}\int_x^{x+\Delta x}\int_y^{y+\Delta y}\int_z^{z+\Delta z} \psi\ dx\ dy\ dz\ dt/(\Delta t \cdot \Delta x \cdot \Delta y \cdot \Delta z) \tag{2.11}$$

Replacing ψ by $\overline{\psi}+\psi'$ and integrating the model equations over the grid volume $\Delta x\cdot\Delta y\cdot\Delta z$ and time interval Δt corresponding to (2.11), the averaged model equations result.

The averaging is done by assuming that $\overline{\overline{\psi}} = \overline{\psi}$, $\overline{\psi'} = 0$, $\overline{\partial\psi/\partial t} = \partial\overline{\psi}/\partial t$, $\overline{\partial\psi/\partial\dot{x}^i} = \partial\overline{\psi}/\partial\dot{x}^i$ etc. Additionally, for the metric tensor and the Christoffel symbol $\dot{g}^{ij} = \overline{\dot{g}^{ij}}$ and $\dot{\Gamma}^i_{jk} = \overline{\dot{\Gamma}^i_{jk}}$ is assumed. Due to these assumptions the surface heights have to be considered as linear within the averaging interval. Microscale pressure and density variations are neglected due to the Markovian hypothesis (Rotta, 1972). In other words, it is assumed that small turbulent pressure fluctuations p' cause only small density variations ρ'.

In the averaged equations the averages $\overline{\psi}$ of temperature, humidity, concentrations, pressure and density are further decomposed into a mesoscale part $\tilde{\psi}$ and a large–scale part ψ_o. The large–scale part represents an area $\Box x\cdot\Box y$ larger than the mesoscale phenomena of interest. In METRAS PC $\Box x\cdot\Box y$ is identical to the model area.

$$\psi_0 = \int_x^{x+\Box x}\int_y^{y+\Box y} \overline{\psi}\; dx\; dy/(\Box x\cdot\Box y) \tag{2.12}$$

Thus ψ_0 is the (horizontal) average of $\overline{\psi}$ which is constant for the same height above sea level. With respect to topography ψ_0 might change in horizontal direction.

For numerical reasons the mesoscale pressure $\tilde{p}$ is additionally decomposed into p_1 and $p_2 = \tilde{p} - p_1$. Their definition and calculation is described in Sections 2.4 and 2.5. In summary the meteorological variables are composed by:

$$u = \overline{u} + u' \tag{2.13a}$$
$$v = \overline{v} + v' \tag{2.13b}$$
$$w = \overline{w} + w' \tag{2.13c}$$
$$\rho = \rho_0 + \tilde{\rho} \qquad \text{(assumption: } \rho' \ll \tilde{\rho}) \tag{2.13d}$$
$$p = p_0 + p_1 + p_2 \qquad \text{(assumption: } p' \ll \tilde{p}) \tag{2.13e}$$
$$\chi = \chi_o + \tilde{\chi} + \chi' \tag{2.13f}$$

In the next section the approximations applied to the model equations are described.

2.4 Approximations

The model may be applied to large areas with higher resolution in subareas of special interest. To calculate pollutant concentrations with respect to the existing meteorological conditions, the model has to take into account the phenomena of the mesoscale γ and mesoscale β. The choosen approximations should not restrict the applicability of the model within this scale. The hatched areas in Figure 2.3 illustrate the scales of validity of several approximations. They are based on scale analysis of the individual terms in the equation of motion and continuity equation, published by Businger (1982), Martin and Pielke (1983), Schlünzen and Schatzmann (1984) and Wippermann (1981). The hydrostatic approximation ($\partial p/\partial z = -g\rho$) can be applied to phenomena of more than 10 km characteristic horizontal scale L_s. The anelastic approximation ($\nabla \cdot \rho \mathbf{v} = 0$) is valid within the entire mesoscale, while the incompressibility assumption can only be applied to horizontal scales smaller than 20 km. The validity of the geostrophic approximation ($\mathbf{v} = \mathbf{V}_g$) can be assumed only in the macroscale. For phenomena with horizontal scales up to $L_s = 1500$ km it is allowed to take the Coriolis parameter f constant and for smaller scales, i.e. close to the surface and up to about 20 km the Coriolis force can be totally neglected.

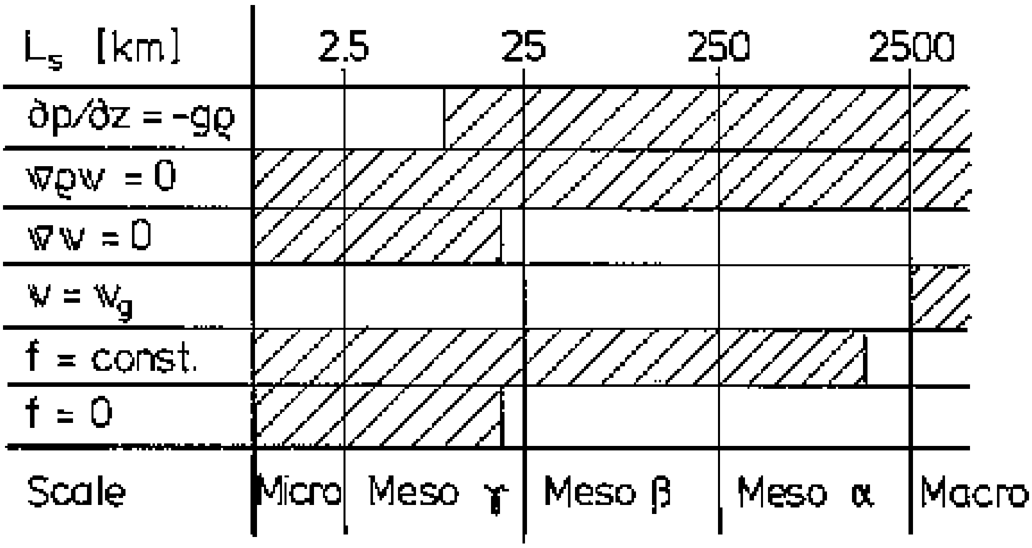

Figure 2.3: Validity range of approximations (hatched areas)

Due to the described validity of approximations and the intended application of METRAS to maximum areas of about 800 x 800 km^2, with horizontal grid increments between some ten meters and 5 km, the model uses the anelastic approximation and a constant Coriolis parameter. The hydrostatic and geostrophic approximation as well as the incompressibility assumption are not valid for this range of application.

The continuity equation in the anelastic approximation is given in η–coordinate system as:

$$\frac{\partial}{\partial \dot{x}^1}\left\{\rho_0 \overset{*}{\alpha}\, \bar{u}\frac{\partial \dot{x}^1}{\partial x}\right\} + \frac{\partial}{\partial \dot{x}^2}\left\{\rho_0 \overset{*}{\alpha}\, \bar{v}\frac{\partial \dot{x}^2}{\partial y}\right\} + \frac{\partial}{\partial \dot{x}^3}\left\{\rho_o \overset{*}{\alpha}\, \overline{\dot{u}^3}\right\} = 0 \qquad (2.14)$$

In approximating (2.9) by (2.14) the validity of the Boussinesq approximation is assumed; deviations of the average density ρ_o can be neglected except for the buoyancy term:

$$\rho = \rho_o \left(1 + \frac{\tilde{\rho}}{\rho_o}\right) \simeq \rho_o \qquad (2.15)$$

Corresponding to (2.13ae) the pressure is decomposed into a large–scale and two mesoscale parts. The large–scale pressure p_o is assumed to fulfill the hydrostatic approximation:

$$\frac{\partial p_o}{\partial \dot{x}^3} = -g\rho_o \frac{\partial z}{\partial \dot{x}^3} \tag{2.16}$$

The large–scale horizontal pressure gradients are shortened in the equations by using the geostrophic approximation. With respect to the used coordinate system $\dot{X}$ this results into:

$$U_g = -\frac{1}{\rho_o f}\left\{\frac{\partial \dot{x}^2}{\partial y}\frac{\partial p_o}{\partial \dot{x}^2} + \frac{\partial \dot{x}^3}{\partial y}\frac{\partial p_o}{\partial \dot{x}^3}\right\} \tag{2.17a}$$

$$V_g = +\frac{1}{\rho_o f}\left\{\frac{\partial \dot{x}^1}{\partial x}\frac{\partial p_o}{\partial \dot{x}^1} + \frac{\partial \dot{x}^3}{\partial x}\frac{\partial p_o}{\partial \dot{x}^3}\right\} \tag{2.17b}$$

The pressure p_1 is calculated by:

$$\frac{\partial p_1}{\partial \dot{x}^3} := -g\rho_o \frac{\tilde{\rho}}{\rho_o}\frac{\partial z}{\partial \dot{x}^3} \tag{2.18}$$

From (2.18) it is obvious that p_1 can be interpreted as the hydrostatic component of the total mesoscale pressure $\tilde{p}$. The mesoscale density deviation $\tilde{\rho}$ for a humid atmosphere can be derived from the linearized gas law (2.19). It is calculated as a function of the mesoscale potential temperature deviation $\tilde{q}_1^1 = \overline{q}_1^1 - {q_o}_1^1$, and liquid water deviations $\tilde{q}_1^2 = \overline{q}_1^2 - {q_o}_1^2$ (Schröder, 1987):

$$\frac{\tilde{\rho}}{\rho_o} = -\frac{\tilde{\theta}}{\theta_o} + \frac{c_v}{c_p}\frac{p_1 + p_2}{p_o} - \left(\frac{R_1^1}{R_o} - 1\right) \cdot \tilde{q}_1^1 + \tilde{q}_1^2 \tag{2.19}$$

c_v and c_p denote the specific heat of dry air at constant volume and at constant pressure, respectively. The large–scale potential temperature θ_o is calculated from

$$\theta_o = T_o \left(\frac{100000}{p_o}\right)^{R/c_p} \tag{2.20}$$

The mesoscale temperature perturbation $\tilde{\theta}$ is calculated from the temperature perturbation $\tilde{T}$ and includes influences of the mesoscale pressure $\tilde{p}$:

$$\tilde{\theta} = \tilde{T}\left(\frac{100000}{p_o + p_1 + p_2}\right)^{R/c_p} \tag{2.21}$$

R_1^1 and R_o are the gas constants of water vapour and dry air. In case of shallow convection the pressure term can be neglected (Dutton, 1976) and $\tilde{\rho}/\rho_o$ can be considered as a function of $\tilde{\theta}/\theta_o$, only. In this case p_1 strongly depends on $\tilde{\theta}$, therefore p_1 is called the 'thermal' pressure part.

In the neutral case, $\tilde{\rho}$ is zero and from (2.18) it can be derived that p_1 remains constant. With $\chi = \theta$, equation (2.10) represents the heat balance and the source term Q_θ includes large–scale heating rates as well as mesoscale and subgrid scale heating rates. For a given stationary and horizontal homogenous situation over flat terrain the local tendencies and horizontal advection of large–scale temperatures θ_o are zero. Only the vertical advection $\bar{w}(\partial\dot{x}^3/\partial z)\cdot(\partial\theta_o/\partial\dot{x}^3)$ remains as a large-scale forcing term. Additional source terms in the heat balance arise from phase changes (Section 3.6) and from radiation flux divergences (Section 3.7).

Replacing χ in (2.10) by the specific humidity $\overline{q}_1^1$ results in an equation for the humidity balance. The pollutant transport equation results from (2.10) if χ is replaced by the concentration C_j of the pollutant j. In METRAS PC only inert tracers are considered.

2.5 Model Equations

Considering the approximations mentioned in the previous section, the model equations of METRAS PC can be compiled now.

The **equations of momentum** are given by:

$$\begin{aligned}
\frac{\partial \rho_0 \overset{*}{\alpha}\, \bar{u}}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{\bar{u}\frac{\partial \dot{x}^1}{\partial x}\rho_0 \overset{*}{\alpha}\, \bar{u}\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{\bar{v}\frac{\partial \dot{x}^2}{\partial y}\rho_0 \overset{*}{\alpha}\, \bar{u}\right\} - \frac{\partial}{\partial \dot{x}^3}\left\{\overline{\dot{u}^3}\rho_0 \overset{*}{\alpha}\, \bar{u}\right\} \\
&\quad - \overset{*}{\alpha}\, \frac{\partial \dot{x}^1}{\partial x}\left\{\frac{\partial p_1}{\partial \dot{x}^1} + \frac{\partial p_2}{\partial \dot{x}^1}\right\} - \overset{*}{\alpha}\, \frac{\partial \dot{x}^3}{\partial x}\frac{\partial p_2}{\partial \dot{x}^3} + \tilde{\rho}\, \overset{*}{\alpha}\, g \frac{\partial \dot{x}^3}{\partial x}\frac{\partial z}{\partial \dot{x}^3} \\
&\quad + f\{\rho_0 \overset{*}{\alpha}\, \bar{v} - \rho_0 \overset{*}{\alpha}\, V_g\} - f' d'\, \rho_0 \overset{*}{\alpha}\, \overline{w} - \overline{F}_1 \qquad (2.22a) \\
\frac{\partial \rho_0 \overset{*}{\alpha}\, \bar{v}}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{\bar{u}\frac{\partial \dot{x}^1}{\partial x}\rho_0 \overset{*}{\alpha}\, \bar{v}\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{\bar{v}\frac{\partial \dot{x}^2}{\partial y}\rho_0 \overset{*}{\alpha}\, \bar{v}\right\} - \frac{\partial}{\partial \dot{x}^3}\left\{\overline{\dot{u}^3}\, \rho_0 \overset{*}{\alpha}\, \bar{v}\right\} \\
&\quad - \overset{*}{\alpha}\, \frac{\partial \dot{x}^2}{\partial y}\left\{\frac{\partial p_1}{\partial \dot{x}^2} + \frac{\partial p_2}{\partial \dot{x}^2}\right\} - \overset{*}{\alpha}\, \frac{\partial \dot{x}^3}{\partial y}\frac{\partial p_2}{\partial \dot{x}^3} + \tilde{\rho}\, \overset{*}{\alpha}\, g \frac{\partial \dot{x}^3}{\partial y}\frac{\partial z}{\partial \dot{x}^3} \\
&\quad - f(\rho_0 \overset{*}{\alpha}\, \bar{u} - \rho_0 \overset{*}{\alpha}\, U_g) + f' d\, \rho_o \overset{*}{\alpha}\, \bar{w} - \overline{F}_2 \qquad (2.22b) \\
\frac{\partial \rho_0 \overset{*}{\alpha}\, \bar{w}}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{\bar{u}\frac{\partial \dot{x}^1}{\partial x}\rho_0 \overset{*}{\alpha}\, \bar{w}\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{\bar{v}\frac{\partial \dot{x}^2}{\partial y}\rho_0 \overset{*}{\alpha}\, \bar{w}\right\} - \frac{\partial}{\partial \dot{x}^3}\left\{\overline{\dot{u}^3}\rho_0 \overset{*}{\alpha}\, \bar{w}\right\} \\
&\quad - \overset{*}{\alpha}\, \frac{\partial \dot{x}^3}{\partial z}\frac{\partial p_2}{\partial \dot{x}^3} + f' \rho_o \overset{*}{\alpha}\, (\bar{u}\, d' - \bar{v}\, d) - \overline{F}_3 \qquad (2.22c)
\end{aligned}$$

The terms $\overline{F}_1$, $\overline{F}_2$, $\overline{F}_3$ are obtained from averaging the equations and describe the subgrid scale turbulent momentum fluxes (see Chapter 3 for their parameterization). The mesoscale pressure p_1 is computed from (2.18), the density $\tilde{\rho}$ from (2.19).

An **equation for the 'dynamic' pressure $\mathbf{p_2}$** has now to be developed. To calculate it, a diagnostic equation can be derived which is based on the following ideas:

- The continuity equation (2.14) has to be fulfilled at every time step.

- The complete equations of motion (2.22) can be integrated by use of the pressure p_2 at the previous time step resulting in velocities $\hat{u}, \hat{v}, \hat{w}$ named 'temporal', which do not fulfill the continuity equation (2.14). The numerical schemes described in Chapter 4 are used for the integration.
- Using the final velocities as given below (Equation (2.23)) in the continuity equation (2.14), a diagnostic elliptic equation for the mesoscale pressure change $\hat{p}_2$ can be derived (Equation (2.24)).

Within this concept the final velocities $\overline{u}^{t+\Delta t}, \overline{v}^{t+\Delta t}$, $\overline{\dot{u}^3}^{t+\Delta t}$ depend on the 'temporal' velocities $\hat{u}, \hat{v}, \hat{\dot{u}}^3$ and the pressure change $p_2^{t+\Delta t} = p_2^t + \hat{p}_2$ in the following way:

$$\bar{u}^{t+\Delta t} = \hat{u} - \frac{1}{\rho_0}\left[\frac{\partial \dot{x}^1}{\partial x}\frac{\partial \hat{p}_2}{\partial \dot{x}^1} + \frac{\partial \dot{x}^3}{\partial x}\frac{\partial \hat{p}_2}{\partial \dot{x}^3}\right]^{t+\Delta t} \cdot \Delta t \tag{2.23a}$$

$$\bar{v}^{t+\Delta t} = \hat{v} - \frac{1}{\rho_0}\left[\frac{\partial \dot{x}^2}{\partial y}\frac{\partial \hat{p}_2}{\partial \dot{x}^2} + \frac{\partial \dot{x}^3}{\partial y}\frac{\partial \hat{p}_2}{\partial \dot{x}^3}\right]^{t+\Delta t} \cdot \Delta t \tag{2.23b}$$

$$\begin{aligned}\overline{\dot{u}^3}^{t+\Delta t} = \hat{\dot{u}}^3 - \frac{1}{\rho_o}\Bigg[&\frac{\partial \dot{x}^1}{\partial x}\frac{\partial \dot{x}^3}{\partial x}\frac{\partial \hat{p}_2}{\partial \dot{x}^1} + \frac{\partial \dot{x}^2}{\partial y}\frac{\partial \dot{x}^3}{\partial y}\frac{\partial \hat{p}_2}{\partial \dot{x}^2} \\ &+ \left(\left(\frac{\partial \dot{x}^3}{\partial x}\right)^2 + \left(\frac{\partial \dot{x}^3}{\partial y}\right)^2 + \left(\frac{\partial \dot{x}^3}{\partial z}\right)^2\right)\frac{\partial \hat{p}_2}{\partial \dot{x}^3}\Bigg]^{t+\Delta t} \cdot \Delta t\end{aligned} \tag{2.23c}$$

The velocities given by Equations (2.23) are used in the continuity equation (2.14) as mentioned above. This results in the following diagnostic elliptic differential equation for the mesoscale pressure $\hat{p}_2$, which denotes the pressure change within time step Δt:

$$\begin{aligned}\nabla \overset{*}{\alpha} \nabla \hat{p}_2 &= \frac{\partial}{\partial \dot{x}^1}\left\{\overset{*}{\alpha}\left(\frac{\partial \dot{x}^1}{\partial x}\right)^2 \frac{\partial \hat{p}_2}{\partial \dot{x}^1} + \overset{*}{\alpha}\frac{\partial \dot{x}^1}{\partial x}\frac{\partial \dot{x}^3}{\partial x}\frac{\partial \hat{p}_2}{\partial \dot{x}^3}\right\} \\ &+ \frac{\partial}{\partial \dot{x}^2}\left\{\overset{*}{\alpha}\left(\frac{\partial \dot{x}^2}{\partial y}\right)^2 \frac{\partial \hat{p}_2}{\partial \dot{x}^2} + \overset{*}{\alpha}\frac{\partial \dot{x}^2}{\partial y}\frac{\partial \dot{x}^3}{\partial y}\frac{\partial \hat{p}_2}{\partial \dot{x}^3}\right\} \\ &+ \frac{\partial}{\partial \dot{x}^3}\Bigg\{\overset{*}{\alpha}\left(\left(\frac{\partial \dot{x}^3}{\partial x}\right)^2 + \left(\frac{\partial \dot{x}^3}{\partial y}\right)^2 + \left(\frac{\partial \dot{x}^3}{\partial z}\right)^2\right)\frac{\partial \hat{p}_2}{\partial \dot{x}^3} \\ &+ \overset{*}{\alpha}\left(\frac{\partial \dot{x}^1}{\partial x}\frac{\partial \dot{x}^3}{\partial x}\frac{\partial \hat{p}_2}{\partial \dot{x}^1} + \frac{\partial \dot{x}^2}{\partial y}\frac{\partial \dot{x}^3}{\partial y}\frac{\partial \hat{p}_2}{\partial \dot{x}^2}\right)\Bigg\} \\ &= \frac{1}{\Delta t}\left[\frac{\partial}{\partial \dot{x}^1}\left\{\rho_0 \overset{*}{\alpha} \hat{u}\frac{\partial \dot{x}^1}{\partial x}\right\} + \frac{\partial}{\partial \dot{x}^2}\left\{\rho_0 \overset{*}{\alpha} \hat{v}\frac{\partial \dot{x}^2}{\partial y}\right\} + \frac{\partial}{\partial \dot{x}^3}\left\{\rho_o \overset{*}{\alpha} \hat{\dot{u}}^3\right\}\right] \\ &= \frac{1}{\Delta t}\nabla(\rho_o \overset{*}{\alpha} \hat{\mathbf{v}})\end{aligned} \tag{2.24}$$

Following equation (2.8), the vertical velocity $\bar{w}$ can be calculated from $\bar{u}, \bar{v}, \bar{\dot{u}}^3$:

$$\bar{w} = \left(\bar{\dot{u}}^3 - \bar{u}\frac{\partial \dot{x}^3}{\partial x} - \bar{v}\frac{\partial \dot{x}^3}{\partial y}\right) \Big/ \frac{\partial \dot{x}^3}{\partial z} \tag{2.25}$$

Momentum divergences resulting from the 'temporal' velocities $\hat{u}, \hat{v}, \overline{\dot{u}}^3$ are balanced by pressure p_2 so that the anelastic approximation (2.14) is fulfilled at every time step. Since p_2 can be different from zero even in a dry atmosphere without mesoscale temperature pertubations, it is called the 'dynamic' pressure.

In the coordinate system $\dot{X}$ the **prognostic equation of the potential temperature** $\tilde{\theta}$ can be written as:

$$\begin{aligned} \frac{\partial \rho_0 \overset{*}{\alpha} \tilde{\theta}}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{\bar{u}\frac{\partial \dot{x}^1}{\partial x}\rho_0 \overset{*}{\alpha} \tilde{\theta}\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{\bar{v}\frac{\partial \dot{x}^2}{\partial y}\rho_0 \overset{*}{\alpha} \tilde{\theta}\right\} \\ &\quad - \frac{\partial}{\partial \dot{x}^3}\left\{(\bar{u}\frac{\partial \dot{x}^3}{\partial x} + \bar{v}\frac{\partial \dot{x}^3}{\partial y} + \bar{w}\frac{\partial \dot{x}^3}{\partial z})\rho_0 \overset{*}{\alpha} \tilde{\theta}\right\} \\ &\quad - \bar{F}_\theta + \rho_0 \overset{*}{\alpha} \overline{Q}_\theta \end{aligned} \tag{2.26}$$

Simulations of a humid atmosphere require additional prognostic equations for water in the different phases. The **balance equation of specific humidity** $\tilde{q}_1^1$ can be written as:

$$\begin{aligned} \frac{\partial \rho_0 \overset{*}{\alpha} \tilde{q_1}^1}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{\bar{u}\frac{\partial \dot{x}^1}{\partial x}\rho_0 \overset{*}{\alpha} \tilde{q_1}^1\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{\bar{v}\frac{\partial \dot{x}^2}{\partial y}\rho_0 \overset{*}{\alpha} \tilde{q_1}^1\right\} \\ &\quad - \frac{\partial}{\partial \dot{x}^3}\left\{(\bar{u}\frac{\partial \dot{x}^3}{\partial x} + \bar{v}\frac{\partial \dot{x}^3}{\partial y} + \bar{w}\frac{\partial \dot{x}^3}{\partial z})\rho_0 \overset{*}{\alpha} \tilde{q_1}^1\right\} \\ &\quad - \bar{F}_{\tilde{q_1}^1} + \rho_0 \overset{*}{\alpha} \overline{Q}_{\tilde{q_1}^1} \end{aligned} \tag{2.27}$$

Replacing $\tilde{q}_1^1$ by $\tilde{q}_1^2$ yields the **balance equation of liquid water**:

$$\begin{aligned} \frac{\partial \rho_o \overset{*}{\alpha} \tilde{q}_1^2}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{\bar{u}\frac{\partial \dot{x}^1}{\partial x}\rho_0 \overset{*}{\alpha} \tilde{q}_1^2\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{\bar{v}\frac{\partial \dot{x}^2}{\partial y}\rho_0 \overset{*}{\alpha} \tilde{q}_1^2\right\} \\ &\quad - \frac{\partial}{\partial \dot{x}^3}\left\{\left(\bar{u}\frac{\partial \dot{x}^3}{\partial x} + \bar{v}\frac{\partial \dot{x}^3}{\partial y} + \bar{w}\frac{\partial \dot{x}^3}{\partial z}\right)\rho_0 \overset{*}{\alpha} \tilde{q}_1^2\right\} \\ &\quad - \bar{F}_{\tilde{q}_1^2} + \rho_0 \overset{*}{\alpha} \overline{Q}_{\tilde{q}_1^2} \end{aligned} \tag{2.28}$$

where $\tilde{q}_1^2$ can be cloud water as well as rain water (see Section 3.6 for details on the parameterization of cloud microphysics).

An analogous equation describes the **balance of pollutant concentrations** $\overline{C}_j$:

$$\begin{aligned} \frac{\partial \rho_0 \overset{*}{\alpha} \tilde{C}_j}{\partial t} &= -\frac{\partial}{\partial \dot{x}^1}\left\{\bar{u}\frac{\partial \dot{x}^1}{\partial x}\rho_0 \overset{*}{\alpha} \tilde{C}_j\right\} - \frac{\partial}{\partial \dot{x}^2}\left\{\bar{v}\frac{\partial \dot{x}^2}{\partial y}\rho_0 \overset{*}{\alpha} \tilde{C}_j\right\} \\ &\quad - \frac{\partial}{\partial \dot{x}^3}\left\{\left(\bar{u}\frac{\partial \dot{x}^3}{\partial x} + \bar{v}\frac{\partial \dot{x}^3}{\partial y} + \bar{w}\frac{\partial \dot{x}^3}{\partial z}\right)\rho_0 \overset{*}{\alpha} \tilde{C}_j\right\} \\ &\quad - \bar{F}_{C_j} + \rho_0 \overset{*}{\alpha} \overline{Q}_{\tilde{C}_j} \end{aligned} \tag{2.29}$$

The terms $\overline{Q}_\chi$ contain the specific sources and sinks for temperature, humidity, liquid water and pollutant concentration as well as their large—scale tendencies. The turbulent flux divergences of $\overline{\chi}$ are summarized in the terms $\overline{F}_\chi$ (Chapter 3). In METRAS PC the subgrid scale fluxes that include χ' are derived from the average values $\overline{\chi}$.

Chapter 3

Parameterization of Subgrid Scale Processes

In this chapter the parameterization of subgrid scale processes including cloud microphysics and radiation is described.

The subgrid scale turbulent transport terms in the model equations are parameterized by a first order closure. It is possible to choose between two alternative approaches to determine the exchange coefficients above the Prandtl–layer (countergradient closure, TKE–ε–closure).

3.1 Subgrid Scale Fluxes of Momentum

The diffusion terms $\overline{F}_i$ in the prognostic equations for momentum can be written as:

$$\begin{aligned}
\overline{F}_1 &= \frac{\partial}{\partial \dot{x}^1}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'u'}\frac{\partial \dot{x}^1}{\partial x}\right\} + \frac{\partial}{\partial \dot{x}^2}\left\{\rho_0 \overset{*}{\alpha}\, \overline{v'u'}\frac{\partial \dot{x}^2}{\partial y}\right\} \\
&+ \frac{\partial}{\partial \dot{x}^3}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'u'}\frac{\partial \dot{x}^3}{\partial x} + \rho_0 \overset{*}{\alpha}\, \overline{v'u'}\frac{\partial \dot{x}^3}{\partial y} + \rho_0 \overset{*}{\alpha}\, \overline{w'u'}\frac{\partial \dot{x}^3}{\partial z}\right\} \qquad (3.1a)
\end{aligned}$$

$$\begin{aligned}
\overline{F}_2 &= \frac{\partial}{\partial \dot{x}^1}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'v'}\frac{\partial \dot{x}^1}{\partial x}\right\} + \frac{\partial}{\partial \dot{x}^2}\left\{\rho_0 \overset{*}{\alpha}\, \overline{v'v'}\frac{\partial \dot{x}^2}{\partial y}\right\} \\
&+ \frac{\partial}{\partial \dot{x}^3}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'v'}\frac{\partial \dot{x}^3}{\partial x} + \rho_0 \overset{*}{\alpha}\, \overline{v'v'}\frac{\partial \dot{x}^3}{\partial y} + \rho_0 \overset{*}{\alpha}\, \overline{w'v'}\frac{\partial \dot{x}^3}{\partial z}\right\} \qquad (3.1b)
\end{aligned}$$

$$\begin{aligned}
\overline{F}_3 &= \frac{\partial}{\partial \dot{x}^1}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'w'}\frac{\partial \dot{x}^1}{\partial x}\right\} + \frac{\partial}{\partial \dot{x}^2}\left\{\rho_0 \overset{*}{\alpha}\, \overline{v'w'}\frac{\partial \dot{x}^2}{\partial y}\right\} \\
&+ \frac{\partial}{\partial \dot{x}^3}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'w'}\frac{\partial \dot{x}^3}{\partial x} + \rho_0 \overset{*}{\alpha}\, \overline{v'w'}\frac{\partial \dot{x}^3}{\partial y} + \rho_0 \overset{*}{\alpha}\, \overline{w'w'}\frac{\partial \dot{x}^3}{\partial z}\right\} \qquad (3.1c)
\end{aligned}$$

The subgrid scale turbulent fluxes, which include u', v', w', can be obtained either by formulating prognostic equations (second order closure) or by deducing them from average velocities. In order to minimize the integration time, the turbulent fluxes in METRAS PC are derived from a first order closure (see e.g. Etling, 1987; Detering, 1985):

$$\tau_{ij} = -\rho_0 \overline{u_i' u_j'} = \rho_0 K_{ij} \left\{ \frac{\partial \bar{u}_i}{\partial x^j} + \frac{\partial \bar{u}_j}{\partial x^i} \right\} \tag{3.2}$$

It should be noted that the reduction of the diagonal fluxes due to pressure (turbulent kinetic energy term) is neglected in METRAS PC since its influence is quite small. The wind components u, v, w in the cartesian coordinate system X are indicated by u_i. In the terrain-following coordinate system $\dot{X}$, equation (3.2) can be written

$$\tau_{ij} = \rho_0 K_{ij} \left\{ \frac{\partial \bar{u}_i}{\partial \dot{x}^k} \frac{\partial \dot{x}^k}{\partial x^j} + \frac{\partial \bar{u}_j}{\partial \dot{x}^k} \frac{\partial \dot{x}^k}{\partial x^i} \right\}, \tag{3.3}$$

where the Einstein summation is used for k ($k = 1, 2, 3$), but not for i and j. For the fluxes τ_{ij} and for the exchange coefficient tensor K_{ij} it can be assumed that they are symmetric with respect to their diagonal, that means $\tau_{12} = \tau_{21}$, $K_{12} = K_{21}$ etc. Besides, identities are assumed for all horizontal and all vertical exchange coefficients:

$$K_{11} = K_{12} = K_{21} = K_{22} = K_{hor} \tag{3.4a}$$

$$K_{13} = K_{23} = K_{31} = K_{32} = K_{33} = K_{vert} \tag{3.4b}$$

This reduces the number of exchange coefficients to be calculated to two values. Therefore, the components τ_{ij} of the turbulent stress tensor can be derived from the gradients of the average variables as follows:

$$\tau_{11} = -\rho_0 \overline{u'u'} = 2\,\rho_0 K_{hor} \left\{ \frac{\partial \overline{u}}{\partial \dot{x}^1} \frac{\partial \dot{x}^1}{\partial x} + \frac{\partial \overline{u}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial x} \right\} \tag{3.5a}$$

$$\tau_{12} = \tau_{21} = -\rho_0 \overline{u'v'} = \rho_0 K_{hor} \left\{ \frac{\partial \overline{u}}{\partial \dot{x}^2} \frac{\partial \dot{x}^2}{\partial y} + \frac{\partial \overline{u}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial y} + \frac{\partial \overline{v}}{\partial \dot{x}^1} \frac{\partial \dot{x}^1}{\partial x} + \frac{\partial \overline{v}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial x} \right\} \tag{3.5b}$$

$$\tau_{13} = \tau_{31} = -\rho_0 \overline{u'w'} = \rho_0\, K_{vert} \left\{ \frac{\partial \overline{u}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial z} + \frac{\partial \overline{w}}{\partial \dot{x}^1} \frac{\partial \dot{x}^1}{\partial x} + \frac{\partial \overline{w}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial x} \right\} \tag{3.5c}$$

$$\tau_{22} = -\rho_0 \overline{v'v'} = 2\rho_0\, K_{hor} \left\{ \frac{\partial \overline{v}}{\partial \dot{x}^2} \frac{\partial \dot{x}^2}{\partial y} + \frac{\partial \overline{v}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial y} \right\} \tag{3.5d}$$

$$\tau_{23} = \tau_{32} = -\rho_0 \overline{v'w'} = \rho_0 K_{vert} \left\{ \frac{\partial \overline{v}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial z} + \frac{\partial \overline{w}}{\partial \dot{x}^2} \frac{\partial \dot{x}^2}{\partial y} + \frac{\partial \overline{w}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial y} \right\} \tag{3.5e}$$

$$\tau_{33} = -\rho_0 \overline{w'w'} = 2\rho_0 K_{vert} \left\{ \frac{\partial \overline{w}}{\partial \dot{x}^3} \frac{\partial \dot{x}^3}{\partial z} \right\} \tag{3.5f}$$

Note that $\frac{\partial \dot{x}^1}{\partial y}$, $\frac{\partial \dot{x}^2}{\partial x}$ etc. are zero. The above formulations are used in both types of turbulence parameterizations. However, when using a counter–gradient closure the fluxes in vertical direction are calculated including deep convection and thus the non–local, counter-gradient transport:

$$\tau_{i3} = \rho_0 K_{vert} \left\{ \frac{\partial \overline{u_i}}{\partial \dot{x}^k} \frac{\partial \dot{x}^3}{\partial x^3} + \frac{\partial \overline{u_3}}{\partial \dot{x}^k} \frac{\partial \dot{x}^k}{\partial x^i} - \Gamma_u \right\} \tag{3.6}$$

3.2 Subgrid Scale Fluxes for Scalar Quantities

The subgrid scale turbulent transport terms of any scalar variable χ (e.g. potential temperature θ) in the coordinate system $\dot{X}$ can be written as

$$\begin{aligned}\overline{F}_\chi &= \frac{\partial}{\partial \dot{x}^1}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'\chi'}\frac{\partial \dot{x}^1}{\partial x}\right\} + \frac{\partial}{\partial \dot{x}^2}\left\{\rho_0 \overset{*}{\alpha}\, \overline{v'\chi'}\frac{\partial \dot{x}^2}{\partial y}\right\} \\ &+ \frac{\partial}{\partial \dot{x}^3}\left\{\rho_0 \overset{*}{\alpha}\, \overline{u'\chi'}\frac{\partial \dot{x}^3}{\partial x} + \rho_0 \overset{*}{\alpha}\, \overline{v'\chi'}\frac{\partial \dot{x}^3}{\partial y} + \rho_0 \overset{*}{\alpha}\, \overline{w'\chi'}\frac{\partial \dot{x}^3}{\partial z}\right\} \qquad (3.7)\end{aligned}$$

The subgrid scale turbulent fluxes $\overline{u_i'\,\chi'}$ are also parameterized by use of a first order closure:

$$\rho_0\, \overline{u_i'\chi'} = \rho_0\; K_{i,\chi}\; \frac{\partial \overline{\chi}}{\partial \dot{x}^k}\frac{\partial \dot{x}^k}{\partial x^i} \qquad (3.8)$$

Similar assumptions as already described for the exchange coefficients of momentum yield:

$$-\rho_0\overline{u'\chi'} = \rho_0 K_{hor,\chi}\left\{\frac{\partial \overline{\chi}}{\partial \dot{x}^1}\frac{\partial \dot{x}^1}{\partial x} + \frac{\partial \overline{\chi}}{\partial \dot{x}^3}\frac{\partial \dot{x}^3}{\partial x}\right\} \qquad (3.9a)$$

$$-\rho_0\overline{v'\chi'} = \rho_0 K_{hor,\chi}\left\{\frac{\partial \overline{\chi}}{\partial \dot{x}^2}\frac{\partial \dot{x}^2}{\partial y} + \frac{\partial \overline{\chi}}{\partial \dot{x}^3}\frac{\partial \dot{x}^3}{\partial y}\right\} \qquad (3.9b)$$

$$-\rho_0\overline{w'\chi'} = \rho_0 K_{vert,\chi}\left\{\frac{\partial \overline{\chi}}{\partial \dot{x}^3}\frac{\partial \dot{x}^3}{\partial z}\right\} \qquad (3.9c)$$

In case of the non–local scheme Equation (3.9c) results in

$$-\rho_0\overline{w'\theta'} = \rho_0 K_{vert,\theta}\left\{\frac{\partial \overline{\theta}}{\partial \dot{x}^3}\frac{\partial \dot{x}^3}{\partial z} - \Gamma_\theta\right\} \qquad (3.10)$$

$$-\rho_0\overline{w'q'} = \rho_0 K_{vert,q}\left\{\frac{\partial \overline{q}}{\partial \dot{x}^3}\frac{\partial \dot{x}^3}{\partial z} - \Gamma_q\right\}, \qquad (3.11)$$

where Γ_θ and Γ_q are the countergradient transport terms. The determination of exchange coefficients and countergradient terms is described in Section 3.4.

3.3 Surface Fluxes

To calculate subgrid scale turbulent fluxes below $z_a \leq 10\ m$, the validity of surface layer similarity theory is assumed. The values of u_*, θ_* and q_* can be calculated with two alternative methods. Both methods consider ten different subgrid scale land use categories (Appendix A), which need to be specified for each grid box by its fraction.

3.3.1 Parameter Averaging

The parameter averaging method uses gridbox–averaged roughness lengths z_0:

$$z_0 = \sum_j f_j \, z_0^j \tag{3.12}$$

f_j is the fraction of the subgrid–scale land use class j within the surface-gridbox and z_0^j the roughness length of the subgrid-scale land use class j.

u_* results from the following equation:

$$u_* = \kappa V(z_{k=1}) \left\{ ln\left(\frac{z_{k=1}}{z_o}\right) - \psi_m\left(\frac{z_{k=1}}{L}\right) \right\}^{-1} \tag{3.13}$$

where $z_{k=1}$ is the height of the lowest model level above the ground. A height of 10 m is recommended for the lowest model level, but lower heights are possible. The velocity $V(z)$ is the surface parallel component of the wind velocity vector. For the calculation of u_* a minimum value of 0.1 m is used for $V(z_{k=1})$. The stability function for momentum $\psi_m(z/L)$ as well as for heat are calculated according to Dyer (1974) with the von Kármán constant κ set equal to 0.4:

$$\psi_m(z/L) = \begin{cases} 2\ln[(1+\Phi_m^{-1})/2] + \ln[(1+\Phi_m^{-2})/2] & \\ \qquad -2\arctan(\Phi_m^{-1}) + \pi/2 & \text{for } z/L \leq 0 \\ -5.0z/L & \text{for } z/L > 0 \end{cases} \tag{3.14}$$

with

$$\Phi_m = \begin{cases} (1-16\ z/L)^{-1/4} & \text{for } z/L \leq 0 \\ 1+5\ z/L & \text{for } z/L > 0 \end{cases} \tag{3.15}$$

The similarity function of heat is assumed as

$$\begin{aligned} \Phi_h &= \Phi_m, \quad \text{for} \quad z/L > 0 \\ \Phi_h &= \Phi_m^2, \quad \text{for} \quad z/L \leq 0. \end{aligned} \tag{3.16}$$

The stability function ψ_h for heat is calculated from:

$$\psi_h(z/L) = \begin{cases} 2\ln\left[\left(1+(1-16.0(z/L))^{\frac{1}{2}}\right)/2\right] & \text{for } z/L < 0 \\ -5.0z/L & \text{for } z/L > 0 \end{cases} \tag{3.17}$$

Equations (3.13) to (3.19) are assumed to be valid in the stability range $-2 \leq z/L \leq 1$.

The Monin-Obukhov-length L is defined by:

$$L = \frac{\overline{\theta} u_*^2}{g\kappa\left[\theta_* + (R_1/R_2 - 1)\overline{\theta} q_*\right]} \tag{3.18}$$

For $|z/L| < 5 \cdot 10^{-3}$ neutral stratification is assumed in the model. The scaling value θ_* for temperature is calculated (e.g. Pielke, 1984) as the scaling values are calculated for other scalars:

$$\chi_* = \kappa \left\{ \overline{\chi}(z_{k=1}) - \overline{\chi}(z_o) \right\} \left(\left[\ln\left(\frac{z_{k=1}}{z_{ok}}\right) - \psi_h\left(\frac{z_{k=1}}{L}\right) \right] \right)^{-1} \tag{3.19}$$

3.3.2 Flux Averaging

The flux averaging method for the calculation of u_* is an application of the concept of blending height (Claussen, 1991; Herrmann, 1994; von Salzen et al., 1996). As a first step, subgrid-scale surface fluxes of momentum ($\sim (u_*^j)^2$), heat ($\sim u_*^j \theta_*^j$) and moisture ($\sim u_*^j q_*^j$) are calculated for each surface class j. At second they are averaged to receive mean surface fluxes which allow to calculate the mean scaling values u_*, θ_* and q_*:

$$u_* = \sqrt{\sum_j f_j \, (u_*^j)^2} \tag{3.20}$$

$$\chi_* = \frac{1}{u_*} \sum_j f_j \, u_*^j \chi_*^j \tag{3.21}$$

The scaling values u_*^j, and χ_*^j of the subgrid-scale surface fluxes are defined as follows:

$$u_*^j = \sqrt{\hat{C}_m^j} \cdot V(z_{k=1}) \tag{3.22}$$

$$\chi_*^j = \frac{\hat{C}_h^j}{\sqrt{\hat{C}_m^j}} \left\{ \overline{\chi}(z_{k=1}) - \overline{\chi}^j(z_0^j) \right\} \tag{3.23}$$

The temperature $\overline{\theta}^j(z_0^j)$ of the subgrid scale surface class j is calculated from a surface energy budget equation (see Section 5.1.2).

An existence of a blending height l_b is assumed. It is defined as the height in which the flow is horizontally homogenous within one grid cell. l_b depends on the roughness and the degree of subgrid-scale heterogenity of the terrain. The effective transfer coefficients $\hat{C}_m^j$ and $\hat{C}_h^j$ are approximated as:

$$\hat{C}_m^j = \frac{\kappa^2}{\left[\ln \frac{l_b}{z_0^j} \frac{\ln(z_p/z_0)}{\ln(l_b/z_0)} - \psi_m\left(\frac{z_p}{L^j}\right) \right]^2} \tag{3.24}$$

$$\hat{C}_h^j = \frac{\kappa^2}{\left[\ln \frac{l_b}{z^j} \frac{\ln(z_p/z_0)}{\ln(l_b/z_0)} - \psi_m\left(\frac{z_p}{L^j}\right) \right] \left[\ln \frac{l_b}{z_{0t}^j} \frac{\ln(z_p/z_{0t})}{\ln(l_b/z_{0t})} - \psi_h\left(\frac{z_p}{L^j}\right) \right]} \tag{3.25}$$

For the height z_p the height of the lowest model level is used ($z_p = z(k = 1)$).

In contrast to the definition of z_0 as weighted average of the roughness lengths z_0^j of the subgrid–scale surface classes (Equation (3.12)), the blending height-roughness length z_0 is now given by:

$$\frac{1}{\left(\ln\frac{l_b}{z_0}\right)^2} = \sum_j \frac{f_j}{\left(\ln\frac{l_b}{z_0^j}\right)^2} \tag{3.26}$$

This equation is solved iteratively together with the following equation, which determines the blending height:

$$\frac{l_b}{l_x}\left(\ln\frac{l_b}{z_0}\right) = c_1\kappa \qquad \text{with } c_1 = 1.75 \tag{3.27}$$

l_x is the characteristic length of subgrid-scale surface elements of even roughness.

The roughness length $z_{0\theta}^j$ for heat of the subgrid-scale surface class j and the mean roughness length $z_{0\theta}$ for heat are calculated from Equation (3.28a), the Monin–Obukhov–Length L^j of class j from Equation (3.18).

3.3.3 Roughness Length

For the different surface characteristics the roughness lenghts for velocity, z_0^j, are prescribed (Appendix A.1). Over water, where the roughness length depends on the wind velocity, it is calculated following Clarke (1970):

$$z_0^0(x,y) = \max\left(0.0185\,u_*^2/g\,,\ \min\left(7\cdot10^{-5}m, \max\left(1.5\cdot10^{-5}m, 0.0032\,u_*^2/g\right)\right)\right) \tag{3.28a}$$

To take into account the differences in exchange processes for momentum, humidity and heat, the ratio of the corresponding roughness lengths is calculated following the results summarized in Hicks (1985). Over surfaces with dense permeable roughness elements (vegetation), the ratio is treated to be constant:

$$\frac{z_0}{z_{0\chi}} = 10. \tag{3.28b}$$

For surfaces with widely spaced bluff roughness elements (urban areas) the ratio of z_0 and $z_{0\chi}$ depends on the roughness Reynolds number $Re_* = u_* z_0/\nu$ (Brutsaert, 1975) with $\nu = 8.788\cdot10^{-3}\cdot\left(\frac{\overline{\Theta}}{10000}\right)^{1.8}$:

$$\frac{z_0}{z_{0\chi}} = \min(\,\exp(\,\kappa\,(7.3Re_*^{1/4}\,\sqrt{SP} - 5))\,,\ 442413) \tag{3.28c}$$

For the calculation of $z_{0\theta}$ the Prandtl number $Pr = 0.71$ has to be used for SP and for z_{0q} the Schmidtnumber $Sc = 0.60$ has to be used for SP. The same calculation is used for water surfaces where waves can develop.

3.4 Exchange coefficients

The exchange coefficients below $z_a \leq 10\ m$ are always calculated form surface layer simularity theory by using the following equations, with Φ_m and Φ_h given in equation (3.15) and (3.14):

$$K_{vert} = \kappa u_* z / \Phi_m \tag{3.29}$$

$$K_{vert,\theta} = K_{vert,q} = \kappa u_* z / \Phi_h \tag{3.30}$$

The determination of exchange coefficients above $z_a = 10$m depends on the type of parameterization used. METRAS PC uses alternatively a non–local scheme given by Lüpkes and Schlünzen, 1996 (Section 3.4.1) or a TKE–ε–closure.

3.4.1 Countergradient Scheme of Lüpkes and Schlünzen (1996)

The nonlocal closure for unstable stratification proposed by Lüpkes and Schlünzen (1996) is based on the prognostic equation of heat flux and on large–eddy simulations of Holtslag and Moeng (1991) and on the scheme proposed by Troen and Mahrt (1986). These parameterizations have been modified to ensure continuity of the turbulent fluxes with respect to height and stratification at a height of $10m$. This requirement results in the following parameterization:

$$K_{vert,\chi} = \frac{\kappa\, u_\star\, z_p}{\left(\Phi_h - \frac{\kappa z_p}{\Theta_\star}\Gamma\Big|_{z_p}\right)} \left(\frac{z_i - z}{z_i - z_p}\right)^2 \frac{u_\star \kappa z + w_f z_i (z/z_i)^{4/3}}{u_\star \kappa z_p + w_f z_i (z_p/z_i)^{4/3}}\,, \quad (z_i \geq z \geq z_p) \tag{3.31}$$

z_p is the height of the first gridlevel.

$$K_{vert} = \left[\frac{\Phi_h\big|_{z_p}}{\Phi_m\big|_{z_p}} + 3\,\frac{w_f u_\star \kappa z_p}{\Phi_m\big|_{z_p}\overline{w'^2}\big|_{z_p} z_i}\right] K_{vert,\chi} \tag{3.32}$$

$$\Gamma_\theta = 3\,\frac{w_f^2 \Theta_f}{\overline{w'^2} z_i} \tag{3.33}$$

The characteristic convective temperature scale is defined by

$$\Theta_f = \frac{\overline{w'\Theta'}\big|_s}{w_f}\,. \tag{3.34}$$

The variance of the vertical velocity $\overline{w'^2}$ is parameterized by

$$(\overline{w'^2})^{3/2} = \left[1.6\, u_\star^2 \left(1 - \frac{z}{z_i}\right)\right]^{3/2} + 1.2 w_f^3 \left(\frac{z}{z_i}\right)\left(1 - 0.9\frac{z}{z_i}\right)^{3/2} \tag{3.35}$$

This formulation is based on large–eddy simulations for convective flow. The second term describes the effect of convection and the first one includes mechanical shear turbulence induced by the surface. Γ_q is given by eq. (3.36):

$$\Gamma_q = \Gamma_\theta \frac{q_\star}{\theta_\star} \tag{3.36}$$

The mixing layer height z_i is determined as the level, where the vertical potential temperature gradient is greater than 0.003 K/m.

The convective velocity scale is given by:

$$w_f = \left(\frac{g}{\Theta_S} z_i \left(\overline{w'\Theta'}\big|_S + (R_1/R_2 - 1)\,\overline{\Theta} \cdot \overline{w'q'}\big|_S \right) \right)^{1/3} \tag{3.37}$$

The mixing length scheme is taken for stable stratification:

$$K_{vert} = \; l_n^2 \left| \frac{\partial v}{\partial z} \right| (1 - 16Ri)^{1/2} \qquad -5 \leq Ri \leq 0 \tag{3.38}$$

and

$$K_{vert,\chi} = \; K_{vert}\,(1 - 16Ri)^{1/4} \qquad -5 \leq Ri \leq 0 \quad . \tag{3.39}$$

The profile functions are similar to those applied by Herbert and Kramm (1985). l_n is the mixing length for neutral stratification, which is specified according to Blackadar (1962) as

$$l_n = \frac{\kappa z}{1 + \frac{\kappa z}{0.007 u_\star / f}} \; . \tag{3.40}$$

The local gradient Richardson number Ri is calculated as follows:

$$Ri = \frac{g}{\overline{\theta}} \; \frac{\left(\frac{\partial \overline{\theta}}{\partial z} + 0.61\, \overline{\theta} \cdot \frac{\partial \overline{q}}{\partial z} \right)}{\left(\left(\frac{\partial \overline{u}}{\partial z} \right)^2 + \left(\frac{\partial \overline{v}}{\partial z} \right)^2 + \zeta \right)} \tag{3.41}$$

The value $\zeta (\approx 10^{-8}/\Delta z^2)$ is added to ensure a nonzero denominator.

3.4.2 TKE–ε–Closure

In METRAS PC a closure of level 2.5 according to the Mellor and Yamada (1974) (MY) classification can be used to calculate the turbulent fluxes of heat, momentum and humidity. The version implemented in METRAS PC combines the original formulation of MY with the nonlocal first order scheme of Lüpkes and Schlünzen (1996) (LS96). For stable and neutral stratification the subgrid scale fluxes are assumed to be proportional to local gradients of the transported quantity. However, in case of unstable stratification counter gradient fluxes of scalar quantities χ are taken into account similar to the LS96 scheme which means that

$$\overline{w'\chi'} = -K_h \left(\frac{\partial \chi}{\partial z} - \Gamma_\chi \right) \ . \tag{3.42}$$

The same parameterizations of the counter gradient terms Γ_χ are used as in the LS96 closure (see Section 3.4.1). The eddy diffusivities for momentum and the energy dissipation rate ε are calculated as function of the turbulent kinetic energy e according to the Heisenberg and Weizsäcker (1946) relations

$$K_{vert} = c_m l \sqrt{\overline{e}} \, ; \qquad \varepsilon = c_m^3 \frac{\overline{e}^{3/2}}{l_\varepsilon} \ , \tag{3.43}$$

where l_ε is the dissipation length scale and l_n is the neutral mixing length

$$l_n = \frac{\kappa z}{1 + \frac{\kappa z}{\lambda}} \ . \tag{3.44}$$

λ is proportional to the boundary layer height z_i:

$$\lambda = a \, z_i, \quad a = 0.08 \, . \tag{3.45}$$

We use the following prognostic equation for the turbulent kinetic energy e

$$\begin{aligned} \frac{\partial}{\partial t}(\overline{e}) + \underbrace{\frac{1}{\rho_0}\frac{\partial}{\partial x_i}(\rho_0 \overline{u_i} \, \overline{e})}_{A} &= \underbrace{K_m \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) \frac{\partial \overline{u_i}}{\partial x_j}}_{M} \underbrace{- \frac{1}{\rho_0}\frac{\partial}{\partial x_3}(\rho_0 \overline{u_3' e})}_{T} \\ &\quad \underbrace{+ \frac{g}{\theta_0} \overline{\theta' u_3'} + 0.61 \, g \, \overline{q' u_3'}}_{B} - \varepsilon \end{aligned}$$

The fluxes of heat and humidity occuring in the bouyancy term B of the e–equation are calculated in case of unstable stratification with Equation (3.42).

The calculation of the mixing length requires the similarity function Φ_m which depends on the Richardson number as in the local first order closure used in METRAS. However, in case of unstable stratification the local Richardson number is replaced by a nonlocal Richardson number defined as

$$Ri_{nl} = \frac{g}{\theta} \frac{\left(\frac{\partial \theta}{\partial z} - \Gamma_\theta + 0.61 \, \theta \left(\frac{\partial q}{\partial z} - \Gamma_q \right) \right)}{\left(\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 + \frac{z}{z_i} \left(\frac{w_f}{z_i} \right)^2 \right)} \tag{3.46}$$

where w_f is the convective velocity scale defined in Equation (3.37).

The eddy diffusivity for heat is calculated by using the same Prandtl number as in the LS96 scheme:

$$K_h = \left[\frac{\phi_h \big|_{z_p}}{\phi_m \big|_{z_p}} + 3 \, \frac{w_f u_\star \kappa z_p}{\phi_m \big|_{z_p} \overline{u_3'^2} \big|_{z_p} z_i} \right]^{-1} K_m \ , \tag{3.47}$$

with the same parameterization of the vertical velocity variance $\overline{u_3'^2}$ as in the LS96 scheme.

For the parameterization of the energy dissipation we use an approach of Therry and Lacarrere (1983)

$$\frac{1}{l_\varepsilon} = \frac{1}{\kappa z} + \frac{C_1}{z_i} - \left(\frac{1}{\kappa z} + \frac{C_2}{z_i}\right) m_1 \, m_2 + \frac{C_5}{l_s} \tag{3.48}$$

$$\begin{aligned} m_1 &= 1/(1 + C_3 z_i/\kappa z) \\ m_2 &= \begin{cases} 1/(1 - C_4 L/z_i) & \text{for} \quad L < 0 \\ 0 & \text{for} \quad L \geq 0 \end{cases} \\ \frac{1}{l_s} &= \begin{cases} 0 & \text{for} \quad \frac{\partial \theta}{\partial z} \leq 0 \\ \left(\frac{g}{\theta_0}\frac{\partial \theta}{\partial z} \Big/ e\right)^{0.5} & \text{for} \quad \frac{\partial \theta}{\partial z} > 0 \end{cases} \end{aligned} \tag{3.49}$$

Herein C_i are constants with $(C_1, C_2, C_3, C_4, C_5 = 15, 5, 0.005, 1, 1.5)$.

3.5 Horizontal Exchange Coefficients

The horizontal exchange coefficient K_{hor} is set to zero in METRAS PC since the advection scheme and the horizontal filtering applied ensures a sufficient horizontal diffusion.

3.6 Parameterization of Cloud Microphysics

Microphysical processes of cloud and rain formation are parameterized in METRAS PC by following the suggestions first presented by Kessler (1969). The Kessler scheme is based on the idea that the liquid water in the atmosphere can be classified in cloud water with a mean droplet radius of about 10 μm and rain water with a mean droplet radius of about 100 μm. Both classes are separated by $r \simeq 40$ μm. The size distribution of the rain water can be described by the Marshall-Palmer distribution (Marshall and Palmer, 1948).

The parameterization scheme includes

- condensation of water vapour to cloud water,
- evaporation of cloud water to water vapour,
- autoconversion of cloud water to rain water by collision of cloud droplets,
- conversion of cloud water to rain water by collection of cloud droplets (accretion),

- sedimentation of rain water and
- evaporation of falling rain drops in sub–saturated layers below clouds.

Since rain–drop–growth by condensation and sedimentation of cloud droplets is of minor importance, these processes are neglected in the parameterization scheme. With this type of parameterization it is necessary to solve two additional prognostic equations of the type (2.28), one for cloud water and one for rain water. Both equations and the prognostic equations for specific humidity and potential temperature are coupled by source/sink terms that include the processes listed above.

Due to the restriction to only two additional prognostic equations and the comparatively simple representation of cloud microphysics this parameterization requires an acceptable amount of computer resources. Nevertheless, it describes the most important processes of cloud and rain formation in a satisfactory way. It is well known, however, that the Kessler scheme tends to overestimate the autoconversion and accretion processes in the early stage of cloud formation resulting in overestimated initial rain rates (e.g. Lüpkes, 1991).

The phase changes of water vapour to cloud droplets and reverse due to condensation and evaporation are calculated by the method of saturation adjustment (Asai, 1965). The values of a variable $\overline{\chi}$ at the next time step $n+1$ are obtained by $\overline{\chi}^{n+1} = \hat{\chi}^{n+1} + \Delta\chi$, where $\hat{\chi}^{n+1}$ denotes a 'temporal' value between time step n and $n+1$ due to advection and diffusion only. The temporal changes of specific humidity Δq_1^1, cloud water content $\Delta q_1^{2\,c}$ and potential temperature $\Delta\theta$ are given by

$$\Delta q_1^1 = \begin{cases} 0 & \text{for } \hat{q}_1^1 < \hat{q}_1^{1sat}(\hat{\theta}) \text{ and } \hat{q}_1^{2c} = 0 \\ \min\left\{-\frac{1}{\beta}(\hat{q}_1^1 - \hat{q}_1^{1sat}(\hat{\theta})), \hat{q}_1^{2c}\right\} & \text{else} \end{cases} \tag{3.50}$$

$$\Delta q_1^{2c} = -\Delta q_1^1 \tag{3.51}$$

$$\Delta\theta = -\frac{l_{21}\cdot\Delta q_1^1}{c_p\cdot\Pi_o} \tag{3.52}$$

where $\hat{q}_1^{1sat}(\hat{\theta})$ denotes the specific saturation humidiy at $\hat{\theta}$, $l_{21} \simeq 2.5\cdot10^6$ J/kg the latent heat of vaporization and $\Pi_o = (p_o/1000\,\text{hPa})^{R/c_p}$ the Exner function. The function β in (3.50) is given by

$$\beta = 1 + \frac{l_{21}\cdot\hat{q}_1^{1sat}(\hat{\theta})\cdot 4028}{c_p\cdot(\hat{\theta}\Pi_o - 38.33)^2} \tag{3.53}$$

The autoconversion of cloud droplets to rain drops starts when the cloud water content exceeds the critical value $q_{1cri}^{2c} = 10^{-3}\ kg/kg$. For larger values the autoconversion rate rises linear with the cloud water content:

$$\left.\frac{\overline{q}_1^{2r}}{\partial t}\right|_{Au} = \begin{cases} k \cdot (\hat{q}_1^{2c} - q_{1cri}^{2c}) & \text{for } \overline{q}_1^{2c} > q_{1cri}^{2c} \\ 0 & \text{else} \end{cases} \tag{3.54}$$

$$\Delta q_1^{2c} \quad = \quad -\,\Delta q_1^{2r} \tag{3.55}$$

The time constant in (3.54) is set up to $k = 10^{-3}\ s^{-1}$.

The accretion rate depends on the probability that rain drops collect cloud droplets during their fall through cloud layers. This probability can be expressed by the so-called collection efficiency. Within the considered concept of warm rain, the assumption of a constant collection efficiency $E = 1$ is justified (Doms and Herbert, 1985). The changes in rain and cloud water content per time step can be written

$$\left.\frac{\partial \overline{q}_1^{2r}}{\partial t}\right|_{Ak} = \sqrt{\frac{\rho_s}{\rho_o}} \cdot 934.63 \cdot \hat{q}_1^{2c} \cdot (10^{-3} \cdot \rho_o \cdot \hat{q}_1^{2r})^{0.875} \tag{3.56}$$

$$\Delta q_1^{2c} = -\,\Delta q_1^{2r} \tag{3.57}$$

where the term $\sqrt{\rho_s/\rho_o}$ with a reference density $\rho_s = 1.29$ kg/m^3 ensures the applicability of (3.56) also to deep convection.

With the assumption of a Marshall–Palmer rain drop size distribution the sedimentation flux of rain is taken into account by

$$\Delta q_1^{2r} = \frac{\Delta t}{\rho_o} \cdot \frac{\partial}{\partial z}(V_{TR} \cdot \rho_o \cdot \hat{q}_1^{2r}) \tag{3.58}$$

where

$$V_{TR} = \sqrt{\frac{\rho_s}{\rho_o}} \cdot 29.13(10^{-3} \cdot \rho_o \cdot \hat{q}_1^{2r})^{0.125} \tag{3.59}$$

denotes the terminal velocity of rain drops. In Equation (3.59) $\sqrt{\rho_s/\rho_o}$ represents the height dependence of V_{TR} due to density changes with height.

When rain drops fall through sub–satured layers below clouds they may evaporate again. This process depends on the sub–saturation as well as on the rain drop size distribution and terminal velocity, expressed in the term A_t and a ventilation factor F_v, respectively:

$$\Delta q_1^{2r} = -\max\left\{\hat{q}_1^{2r}\ \frac{10^3 \cdot \Delta t}{\rho_o} \cdot A_t \cdot \sqrt{10^{-3}\rho_o \hat{q}_1^{2r}} \cdot F_v \cdot S\right\} \tag{3.60}$$

$$\Delta q_1^1 = -\Delta q_1^{2r} \tag{3.61}$$

$$\Delta\theta = -\frac{l_{21}}{c_p \cdot \Pi_o} \cdot \hat{q}_1^{2r} \tag{3.62}$$

with

$$A_t = \frac{2.623 \cdot 10^{-3}(10^{-3} \cdot \rho_o \cdot \hat{q}_1^{1sat}(\hat{\theta}))}{1 + 1.282 \cdot 10^{10}(10^{-3} \cdot \rho_o \cdot \hat{q}_1^{1sat}(\hat{\theta})) \cdot \hat{T}^{-2}} \qquad (3.63)$$

characterizing the rain drop spectra and

$$F_v = 0.78 + 80.73 \cdot (10^{-3} \cdot \rho_o \cdot \hat{q}_1^{2r})^{0.225}. \qquad (3.64)$$

The subsaturation is given by

$$S = \frac{\hat{q}_1^{1sat}(\hat{\theta}) - \hat{q}_1^1}{\hat{q}_1^{1sat}(\hat{\theta})} \cdot 100 \qquad (3.65)$$

It should be pointed out that, unlike to this chapter, most literature on cloud physics give the formulars in cgs-units. For clarity, all equations listed above refer to SI-units, resulting in a number of additional factors 10^{-3}. Further details on the parameterization of cloud microphysics in METRAS PC are given by Köhler (1990).

3.7 Parameterization of Radiation

Two alternative parameterizations for radiative fluxes are implemented in METRAS PC to take into account the heating and cooling of the surface and atmosphere due to the net radiation. If a simulation without cloud formation is performed, only the longwave and shortwave radiation budgets at the earth's surface are computed. This computation is carried out with respect to the geographical position, date and time, rotation of the coordinate system against North, surface inclination, and shading of areas due to neighbouring mountains. Details on this parameterization are given in Section 5.1.2 and Appendix A.2.

In the atmosphere an empirical formulation is used for the cooling rates: At the surface during daytime the cooling amounts to 2 K/day while it is 3 K/day at nighttime. The cooling rate decreases exponentially with height:

$$\left.\frac{\partial T}{\partial t}\right|_{rad} = -\text{cooling rate } [K/s] \cdot e^{-(z-z_0)/600} \qquad (3.66)$$

In case of model calculations with the formation of clouds, the radiation fluxes at the earth's surface and in the atmosphere are parameterized by use of a two–stream approximation scheme. This scheme takes into account absorption and reflection of longwave and shortwave radiation by water vapour and liquid water and leads to cooling or heating not only at the surface but also at each grid point above. Here the basic ideas of the scheme are described, which is given by Bakan (1994).

The cooling rate at a grid point k (counting in the vertical direction) due to longwave radiation flux divergences is given by

$$\left.\frac{\partial \overline{T}}{\partial t}\right|_k^{rad} = -\frac{1}{\rho_0 c_p} \left.\frac{dF_N}{dz}\right|_k \tag{3.67}$$

with the radiation flux

$$F_N|_k = F_\uparrow^+ - F_\uparrow^- + F_\downarrow^- - F_\downarrow^+ \tag{3.68}$$

where '+' and '-' denote locations at the upper and lower boundary of the grid volume k, respectively. With B the Planck function, σ a volume absorption coefficient and $\beta = 1.66$ a diffusivity parameter, the up– and downward fluxes can be written as

$$F_\uparrow^+ = F_\uparrow^- \cdot e^{-\beta\sigma\Delta z} + B^+ - B^- \cdot e^{-\beta\sigma\Delta z} - \frac{B_z}{\beta\sigma}(1 - e^{-\beta\sigma\Delta z}) \tag{3.69a}$$

$$F_\downarrow^- = F_\downarrow^+ \cdot e^{-\beta\sigma\Delta z} + B^- - B^+ \cdot e^{-\beta\sigma\Delta z} - \frac{B_z}{\beta\sigma}(1 - e^{-\beta\sigma\Delta z}) \tag{3.69b}$$

For shortness B_z means the vertical gradient of B. Equations (3.69a, 3.69b) are separately solved for different spectral ranges.

Within the atmospheric window ($8.33 - 11.11\ \mu m$) absorption by liquid water is the dominant process. The absorption coefficient for liquid water is taken following Buykov and Khvorostyanov (1977)

$$\sigma_l = 50 \cdot \rho_0(\overline{q}_1^{2c} + \overline{q}_1^{2r}) \tag{3.70}$$

and for water vapour

$$\sigma_v = 1.38 \cdot \rho_0 \cdot (\overline{q}_1^1)^2 \cdot \frac{\overline{p}}{p_o} \cdot e^{\left(\frac{1800}{\overline{T}} - 6.08\right)} \tag{3.71}$$

where p/p_o takes into account the pressure dependency of the absorption. The Planck function can be written as

$$B_{win} = \pi[88.75 - 0.9706 \cdot \overline{T} \cdot (1 - 0.002851 \cdot \overline{T})] \tag{3.72}$$

Instead of a detailed description of the CO_2 absorption between 13 and $18 \mu m$ the black body irradiance of CO_2 is parameterized by

$$B_{CO_2} = \pi[10.63 - 0.1679 \cdot \overline{T} \cdot (1 - 0.004025 \cdot \overline{T})] \tag{3.73}$$

Outside of the $8.33 - 11.11\ \mu m$ and $13 - 18\ \mu m$ range, spectral absorption by water vapour is dominant. Since it strongly depends on the wavelength, the transmission function is expanded into a sum of exponential functions with separate absorption coefficients of different weights

$$\sigma_v^i = 10^3 \cdot \rho_0 \cdot \overline{q}_1^1 \cdot \frac{\overline{p}}{p_o} \cdot \tilde{\sigma}_v^i \quad i = 1, 8 \tag{3.74}$$

i	1	2	3	4
$\tilde{\sigma}_v^i$ $[m^2/kg]$	$4.285 \cdot 10^{+1}$	$6.053 \cdot 10^{\pm 0}$	$8.550 \cdot 10^{-1}$	$1.208 \cdot 10^{-1}$
i	5	6	7	8
$\tilde{\sigma}_v^i$ $[m^2/kg]$	$1.706 \cdot 10^{-2}$	$2.410 \cdot 10^{-3}$	$3.404 \cdot 10^{-4}$	$4.808 \cdot 10^{-5}$

Table 3.1: Volume absorption coefficients of water vapour

where $\tilde{\sigma}_v$ denotes the volume absorption coefficient of water vapour as given in Table 3.1.

In practice the range $i = 8$ can be negelected due to its minor weight.

Subtracting the Planck function for the atmospheric window and the CO_2 range yields

$$B_{out} = \sigma \overline{T}^4 - B_{win} - B_{CO_2} \tag{3.75}$$

where $\sigma = 5.67032 \cdot 10^{-8}\ Wm^{-2}K^{-4}$ is the Stefan–Boltzman constant.

The downward solar radiation flux can be written as a product of several transmission factors:

$$E = E_o \cdot \mu \cdot T_E \cdot T_V \cdot T_D \cdot T_L \cdot f_A \tag{3.76}$$

where E_o denotes the solar constant, $\mu = \cos Z(t)$ with $Z(t)$ the zenith angle (see Appendix A.2), f_A is a function of Albedo and T are transmission factors due to Rayleigh scattering (T_E), absorption by water vapour (T_V), absorption and scattering by aerosols (T_D) and liquid water (T_L). Equation (3.76) is separately calculated for the visible range 1 ($\lambda < 0.75\mu m$) and a near infrared range 2 ($\lambda > 0.75\mu m$). Within the radiation module of METRAS PC $T_{E2} = T_{V1} = T_{D1} = f_{A1} = f_{A2} = 1$ is assumed. The solar constants of both ranges are taken as $E_{o1} = 707W/m^2$ and $E_{o2} = 660W/m^2$.

The transmission factor for Rayleigh scattering is derived from a suggestion of Atwater and Brown (1974) (Bakan, 1994)

$$T_{E1} = 1.041 - 0.16\sqrt{\frac{0.962 \cdot \overline{p}/p_o + 0.051}{\mu}} \tag{3.77}$$

and scattering by liquid water is parameterized following Stephans et al. (1984)

$$T_{L1} = \frac{1}{1 + \beta_1 \tau_{N1}/\mu} \tag{3.78}$$

where $\beta_1 = 0.08\sqrt{\mu}$ is the backscattering fraction, $\tau_{N1} = 1.8336\ (log_{10} W_L)^{3.963}$ the optical thickness of a cloud, and $W_L = 10^3 \int_z^\infty \rho_0(\overline{q}_1^{2c} + \overline{q}_1^{2r})dz[g/m^2]$ the liquid water mass above the location under consideration.

In the near infrared, absorption by water vapour is given by

$$T_{V2} = 1 - 0.193(W_V/\mu)^{0.37} \tag{3.79}$$

with

$$W_V = 10^{-1} \int_z^\infty \frac{\overline{p}}{p_0} \cdot \rho_0 \cdot \overline{q}_1^1 dz [g/m^2] \tag{3.80}$$

being the mass of water vapour analogous to W_L. As in (3.71) and (3.74) the factor $\overline{p}/p_o$ takes the pressure dependency of the absorption into account. The transmission factor for liquid water is formulated following Stephans et al. (1984):

$$T_{L2} = 4 \cdot \mu/R \tag{3.81}$$

with

$$\begin{aligned}
R &= (u+1)^2 \cdot e^{\tau_{eff}} - (u-1)^2 e^{-\tau_{eff}} \\
\tau_{eff} &= \frac{\tau_{N2}}{\mu}\sqrt{(1-\omega)(1-\omega+2\beta_2\omega)} \\
u^2 &= \frac{1-\omega+2\beta_2\omega}{1-\omega} \\
\tau_{N2} &= 2.2346\,(log_{10} W_L)^{3.8034} \\
\omega &= 1 - 0.004 \cdot \mu^2 \cdot ln\,(500/\tau_N) \\
\beta_2 &= 0.12 \cdot \sqrt{\mu}/ln\,(3 + \tau_N/10) \\
\tau_N &= \tau_{N2}(W_L(z=0))
\end{aligned}$$

The corresponding reflectivity is calculated from

$$R_{L2} = (e^{\tau_{eff}} - e^{-\tau_{eff}})\frac{u^2-1}{R} \tag{3.82}$$

Chapter 4

Numerical Treatment

In this chapter the numerical schemes used for solving the discretized model equations as well as the used grid are presented.

4.1 Non–uniform Grid

The model equations are spatialy discretized on an ARAKAWA–C–grid, which represents gravity waves better than other grids (Mesinger and Arakawa, 1976). From Figure 4.1 it can be seen that the components of the velocity vector are defined at grid points which are apart from the grid point for scalar variables. The displacement of the velocity components by half of the grid size increases the accuracy of the used numerical methods for the computation of divergencies. Some of the transformation coefficients, used to discretize the equations, are defined at scalar grid points, others are defined at vector grid points.

Figure 4.2 shows a projection of scalar and vector grid points to the horizontal $\dot{x}^1, \dot{x}^2$ plane (left) and the vertical $\dot{x}^1, \dot{x}^3$ plane (right). The lateral boundaries of the model area are defined at $i = j = 0.5$, corresponding to the index 0 of the vector field, and $i = NX1 + 0.5$, $j = NX2 + 0.5$, corresponding to the index NX1 and NX2 of the vector field. The surface boundary lies at $k = 0.5$ and the model top boundary at $k = NX3 + 0.5$. The velocity components are defined at these boundaries with respect to the direction they represent (i.e. u at $\dot{x}^1$-boundaries, v at $\dot{x}^2$-boundaries, w at $\dot{x}^3$-boundaries), whereas the boundary values of scalar variables are calculated at half a grid width outside of the model area. The same holds for velocity components in those directions, where they are defined at scalar grid points. This grid representation enables the coupling of velocity and pressure arrays at the boundaries (see Section 5.3).

Figure 4.3 shows the grid representation for a non–uniform grid. The model equations

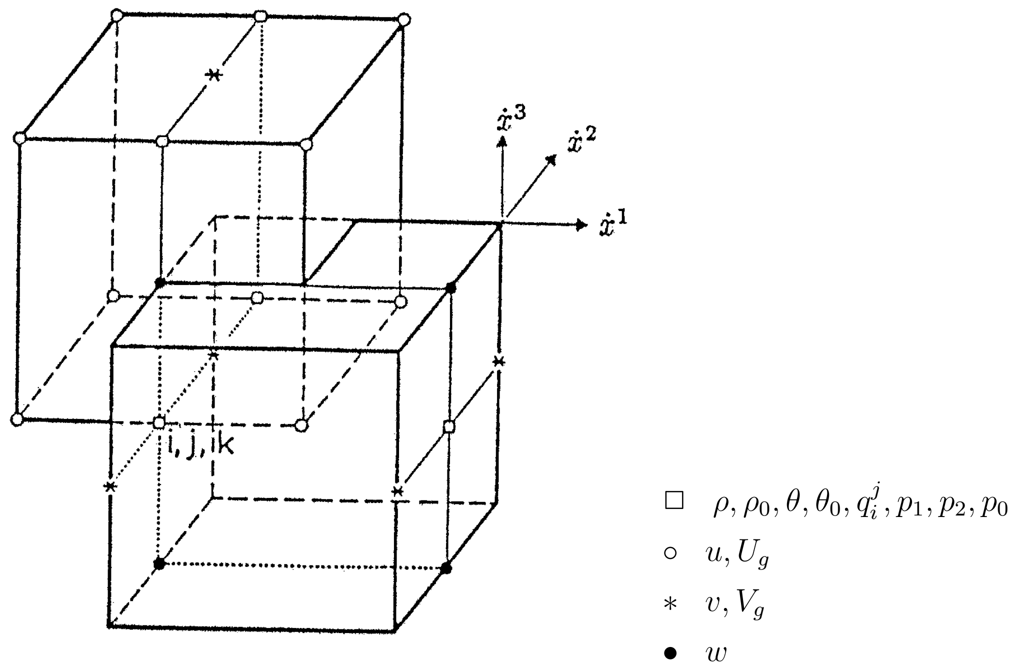

Figure 4.1: Three–dimensional grid representation in METRAS (ARAKAWA–C)

are transformed and solved in a uniform grid with uniform grid increments $\Delta\dot{x}^1 = \Delta\dot{x}^2 = \Delta\dot{x}^1 = 1$ ($\Delta\dot{x}^1, \Delta\dot{x}^2, \Delta\dot{x}^3$ without unit). The coordinates of scalar grid points in the coordinate system $\dot{X}$ are defined as follows:

$\dot{x}^1 = \mathrm{i}$ with $i = 0, 1, \ldots$ NX1 + 1, resulting in NX1+2 gridpoints
$\dot{x}^2 = \mathrm{j}$ with $j = 0, 1, \ldots$ NX2 + 1, resulting in NX1+2 gridpoints
$\dot{x}^3 = \mathrm{k}$ with $k = 0, 1, \ldots$ NX3 + 1, resulting in NX1+2 gridpoints

The vector grid points are defined in a similar way. It follows that there are $NX1 + 1$ vector u–points in direction $\dot{x}^1$, $NX2 + 1$ vector v–points in direction $\dot{x}^2$ and $NX3 + 1$ vector w–points in direction $\dot{x}^3$.

4.2 Temporal Integration Scheme of the Model

The solving of the model equations follows the temporal integration scheme given in Figure 4.4.

After specifying initial values for all variables the integration within the time loop starts within the initalization phase with the computation of new surface heights (diastrophism).

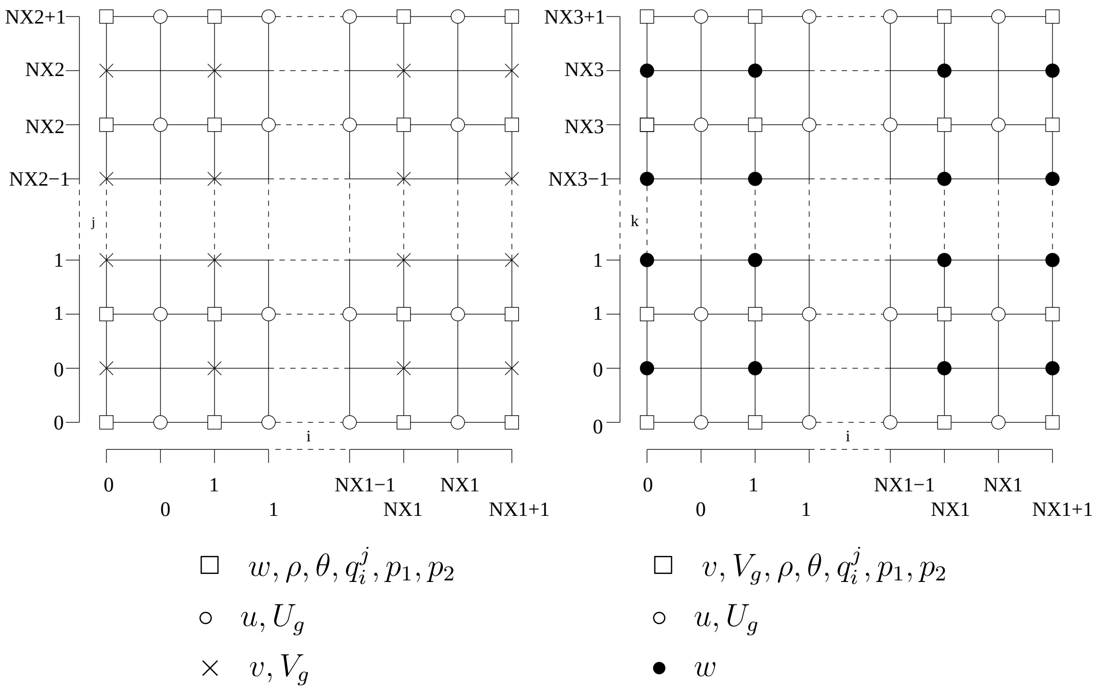

Figure 4.2: Grid representation in a $\dot{x}^1, \dot{x}^2$ plane (left) and $\dot{x}^1, \dot{x}^3$ plane (right)

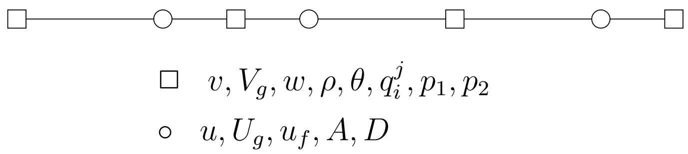

Figure 4.3: Grid representation in $\dot{x}^1$–direction

As a next step the friction velocity u_*, temperature scale θ_*, and the humidity scale q_* are determined by iteration and the exchange coefficients are derived. The wind components and mesoscale pressure p_2 are computed for the new time step. With the new wind fields and exchange coefficient values the equations for the scalar variables temperature, humidity, liquid water and pollutants are solved in a semi–implicit manner. Finally, the mesoscale density $\tilde{\rho}$ and pressure p_1 are derived from diagnostic equations.

Without using the new wind fields for solving the equations of temperature and humidity it would be necessary to adapt the time step to the speed of gravity waves which can reach 300 m/s. The use of huge amounts of computation time can be avoided by using the semi–implicit integration scheme (Pielke, 1984). The balance equations of liquid water and pollutants are also solved semi–implicit, which is not necessary but reduces memory resources because no additional auxiliary arrays for temporal velocity fields are required.

Specification of initial values	
Time integration loop	
	Calculation of corresponding time
	If specified: topography 'diastrophy'
	Calculation of exchange coefficients and surface characteristics
	Calculation of wind field, pressure p_2
	If specified: calculation of scalar quantities $(\tilde{\theta}, \tilde{q_1^2}, \tilde{C}_j)$
	Calculation of density $\tilde{\rho}$
	Calculation of pressure p_1
	If specified: OUTPUT of selected values
End of simulation	

Figure 4.4: Integration scheme of model METRAS PC

4.3 Numerical Schemes

The numerical schemes implemented in METRAS PC have been choosen with regard to the requirements that they

- require a minimum of computer memory,
- can easily be vectorized for optimization,
- supply convergent and stable solutions and
- have low numerical diffusion.

Due to nonlinear instability of the model equations the solutions can be disturbed by the formation of $2\Delta x$-waves (Haltiner and Williams, 1980). To avoid such instabilities, filters are implemented in METRAS PC with three levels of diffusity to damp $2\Delta x$–waves (Shapiro, 1971).

Level 1 (3 point):

$$\ddot{\psi}_i = \frac{1}{4} \cdot (\psi_{i+1} + 2 \cdot \psi_i + \psi_{i-1}) \qquad (4.1)$$

Level 2 (5 point):

$$\ddot{\psi}_i = \frac{1}{16} (-\psi_{1+2} + 4\psi_{i+1} + 10\psi_i + 4\psi_{i-1} - \psi_{i-2}) \qquad (4.2)$$

Level 3 (7 point):

$$\ddot{\psi}_i = \frac{1}{64}\left(\psi_{i+3} - 6\psi_{i+2} + 15\psi_{i+1} + 44\psi_i + 15\psi_{i-1} - 6\psi_{i-2} + \psi_{i-3}\right) \tag{4.3}$$

ψ represents unfiltered values and $\ddot{\psi}$ filtered values. Boundary values remain unfiltered. The 7 point filter (4.3) is applied in METRAS PC in horizontal direction, resulting in low damping. Towards the lateral boundaries, the 5 point or 3 point filter is used which are more diffusive but minimize boundary value problems.

The filters are only used in horizontal direction for wind, temperature and humidity, at first in x– and at second in y–direction. For radiational heating and cooling, calculated as described in Section 3.7, the filter (4.1) is used in vertical direction. This implicitly considers the intense vertical mixing processes occuring in clouds.

4.3.1 Solution of the Equation of Motion

The temporal discretization of the advection terms follows the Adam–Bashforth scheme. Spatial derivatives are approximated by centered differences. This scheme is slightly unstable, but the typical computational mode of 3–level–schemes is damped (Mesinger and Arakawa, 1976). Following Schumann (1983), this scheme is stable for solving the equations of motion, if, as it is done in METRAS PC, the diffusion terms are also calculated with this scheme. To increase the time step for vertical exchange processes an implicit scheme (Crank Nicholson) is implemented to solve vertical diffusion.

The Coriolis and gravity terms of the equation of motion are discretized forward–in–time and centered–in–space. Although forward–in–time differences of the Coriolis terms may leed to instabilites (e.g. Kapitza, 1987), this method can be used due to the very small amplification of waves, when time steps shorter than $100sec$ are used (Pielke, 1984). In METRAS PC time steps are limited to $60sec$.

The gradients of the mesoscale pressure p_2 are solved implicit with backward differences. By doing so the anelastic assumption (2.14) is achieved at every time. The pressure gradients are discretized centered-in-space, as is done with all other gradients not mentioned here. All variables which are not defined at the grid points where they are used, are taken as an average from the neighbouring grid points.

4.3.2 Solution of Scalar Equations

The advection terms are discretized by the well known upstream scheme. The exchange processes can be solved forward–in–time and centered–in–space or, alternatively, for the vertical direction with the implicit Crank–Nicholson–scheme.

4.3.3 Solution of the Diagnostic Equations

The mesoscale pressure p_1 can be subsequently computed by numerical integration of (2.18) from the upper model boundary to the ground. The mesoscale density deviation $\tilde{\rho}$ is derived from the diagnostic equations (2.19) as a function of the mesoscale temperature deviation $\tilde{\theta}$ and the mesoscale pressure $\tilde{p} = p_1 + p_2$. Since the pressure p_1 at time step $n + 1$ is unknown (see Figure 4.4), the known value at time step n is used. However, for the temperature and the mesoscale pressure p_2 the values at time step $n+1$ are used. The density $\tilde{\rho}(k, j, i)$, therefore, is derived semi-implicit. Additional boundary values are only necessary for p_1 at the model top, where $p_1 = 0$ is assumed and all pressure deviations are summarized in the pressure p_2.

Equation (2.24) for the mesoscale pressure p_2 is an elliptic differential equation, which can be solved directly or by an iterative procedure. Within METRAS PC the iterative IGCG–scheme (**I**dealized **G**eneralized **C**onjugate **G**radient; Kapitza and Eppel, 1987) is used.

Chapter 5

Boundary Conditions

The model area is limited in vertical and horizontal directions. Over land the surface height z_s and over water the water surface coincide with the lower model boundary. The remaining five boundaries are artificial in the sense that they do not correspond to natural boundaries between two media. Therefore, the corresponding boundary conditions need to be formulated in such a way that waves can pass these boundaries without reflection.

In METRAS PC the boundary conditions are based on the following assumptions:

1. Lateral boundaries can be inflow and outflow boundaries at the same time.
2. Boundary values of the wind components $\overline{u^1}$, $\overline{u^2}$, $\overline{u^3}$ normal to the boundary are coupled to the mesoscale pressure p_2. The boundary conditions take this relation into account, as it is done in other mesoscale models (Clark, 1977; Schumann and Volkert, 1984).
3. The grid widths $\Delta x, \Delta y$ remain constant for the first three scalar grid points, including the scalar grid point outside the model area. Thus the derivatives $\partial \dot{x}^1 / \partial x$ at the west/east boundaries and $\partial \dot{x}^2 / \partial y$ at the south/north boundaries remain constant for two vector grid points.
4. The increment Δz remains constant for the three lowest and highest scalar grid points, including the scalar grid point below the surface and above the model top. Thus the derivative $\partial \dot{x}^3 / \partial z$ remains constant for two vector grid points.
5. The surface heights z_s remain constant normal to the boundaries for three scalar grid points, which yields $\partial \dot{x}^3 / \partial x = 0$ and $\partial \dot{x}^3 / \partial y = 0$ for two vector points at the corresponding lateral boundaries.

These five assumptions do not limit the range of applicability of the mesoscale model. Within checked limits (see Schlünzen (1988), Section 5.1) the grid increments can be chosen without reducing the solvability of the equation system. The grid increments can be chosen depending on the requirements of the application. The constant surface heights prescribed at the lateral boundaries differ form reality. However, prognosed variables should never be interpreted near the boundaries due to the artificial character of boundaries. In case of complex terrain (due to land–use or topography), reliable values of the prognostic variables can be assumed about 5 grid points from the lateral boundaries.

The following boundary conditions are derived with respect to the assumptions mentioned above.

5.1 Lower Boundary

Usually the surface is not a flat and homogenous plane, but rough, covered with vegetation (forest, grass, fields) or built-up (houses). From this the question arises, how to determine the height z_s of the lower model boundary. In METRAS PC it is considered as topography height, corresponding to the sum of surface height $h(x,y)$ and roughness length $z_o(x,y)$:

$$z_s(x,y) = h(x,y) + z_o(x,y) \tag{5.1}$$

However, since the roughness lengths are mostly very small, z_0 is neglected when calculating the topography height. Therefore, the lower model boundary corresponds to the orography height ($z_s(x,y) = h(x,y)$). The physical meaning of the lower boundary in the model, however, remains that of the topography height.

5.1.1 Wind and Pressure

The wind velocity at the surface usually follows a no–slip condition, thus the horizontal and vertical wind components are zero at the ground:

$$\bar{u}|_{z_s} = 0 \tag{5.2a}$$

$$\bar{v}|_{z_s} = 0 \tag{5.2b}$$

$$\bar{w}|_{z_s} = 0 \tag{5.2c}$$

Corresponding to equation (2.23c) the boundary condition for the pressure p_2 can be formulated with regard to Equations (5.2a—5.2c):

$$\frac{\partial \dot{x}^1}{\partial x}\frac{\partial \dot{x}^3}{\partial x}\frac{\partial \hat{p}_2}{\partial \dot{x}^1} + \frac{\partial \dot{x}^2}{\partial y}\frac{\partial \dot{x}^3}{\partial y}\frac{\partial \hat{p}_2}{\partial \dot{x}^2} + \left(\left(\frac{\partial \dot{x}^3}{\partial x}\right)^2 + \left(\frac{\partial \dot{x}^3}{\partial y}\right)^2 + \left(\frac{\partial \dot{x}^3}{\partial z}\right)^2\right)\frac{\partial \hat{p}_2}{\partial \dot{x}^3} = 0 \tag{5.3}$$

For the pressure p_1 no boundary value needs to be specified since it is diagnosed from known values of $\tilde{\rho}$ which depends on $\tilde{\theta}$, p_1, $\tilde{q_1^1}$, $\tilde{q_1^2}$. For all these values boundary values are specified.

5.1.2 Temperature

The temperature at the surface can be kept constant during the model run. As an alternative the temperature at the surface can be calculated from a surface energy budget equation:

$$(1-\alpha)(I+D) + L\downarrow - L\uparrow + Q_H + Q_E + Q_S + Q_F = 0 \tag{5.4}$$

Here $(1 - A_0)(I + D)$ characterizes the direct and diffusive short wave radiation budget and can be calculated from the radiation scheme given in Section 3.7, or for more simple purposes, from $\mu I_\infty cosZ(t)$. The parameter μ depends on the albedo A_0, the amount of clouds, the turbidity of the air and the elevation of the sun. For a cloud free sky, μ can be estimated to 0.75 (1 -A_0) for Northern Germany (Golchert, 1981). With a typical value for the albedo A_0 over land, μ results in 0.75 (1 - 0.2) = 0.6. The zenit angle $Z(t)$ is calculated in the model dependent on the terrain slope, time, latitude, etc. (see Appendix A.2).

The incoming and outgoing long wave radiation L can also be calculated with respect to the radiation budget in the atmosphere or, more simple (e.g. for cloud free skies), from $\hat{\varepsilon}\sigma T_s^4$ dependent on the surface temperature T_s, the Stefan-Bolzmann-constant $\sigma = 5.67 \cdot 10^{-8}$ $[W/m^2K^4]$ and the parameter $\hat{\varepsilon}$. The last depends on the amount of clouds and the water content in the atmosphere. Following de Jong (1973) $\hat{\varepsilon} = 0.22$ is used for a cloudfree sky.

The fourth and fivth terms in Equation (5.4) characterize the sensible (Q_H) and latent (Q_E) heat fluxes. They are calculated by the parameter averaging (Section 3.3.1) or the flux averaging method (Section 3.3.2).

Q_s characterizes the heat flux and heat exchange with the deep soil layers and can be calculated from $Q_s = \nu_s(\partial\overline{T}/\partial z)_s$. Within the soil the conduction of heat may be calculated with a one–dimensional diffusion equation:

$$\frac{\partial\overline{T}}{\partial t} = \frac{\partial}{\partial z}\left(k_s\frac{\partial\overline{T}}{\partial z}\right) \tag{5.5}$$

This equation is linearized in METRAS PC by assuming one soil plus vegetation layer. Following Tiedke and Geleyn (1975) and Deardorff (1978), Equation (5.4) is solved by use of the force–restore method, resulting in:

$$\begin{aligned}\frac{\partial\overline{T}_s}{\partial t} = \frac{2\sqrt{\pi}\,k_s}{\nu_s\cdot h}\Big\{&\mu\, I_\infty\, cosZ(t) - \hat{\varepsilon}\sigma\overline{T}_s^4 + c_p\,\rho_0\,\theta_*\,u_* \\ &+ l_{21}\rho_o q_* u_* - \sqrt{\pi}\nu_s\frac{\overline{T}_s - \overline{T}(-h_\theta)}{h_\theta}\Big\}\end{aligned} \tag{5.6}$$

Here k_s is the thermal diffusivity and ν_s the thermal conductivity of the soil. The values used in the model for the different vegetation types are given in Appendix A.1. The depth

h_θ of the daily temperature wave can be calculated following Deardorff (1978) from k_s with $\tau_1 = 86400s$:

$$h_\theta = \sqrt{k_s \cdot \tau_1} \tag{5.7}$$

The temperature in the soil $\overline{T}(-h_\theta)$ is kept constant which is valid for short range forecasts (e.g. a few days).

The real temperature at the surface calculated from equation (5.6) is converted to potential temperature. The boundary value $\overline{\theta}$ (lowest level) is derived from $\overline{\theta}(z_s)$ and $\overline{\theta}$ (first level) with the assumption of constant gradients:

$$\overline{\theta}\text{ (lowest level)} = 2 \cdot \overline{\theta}(z_s) - \overline{\theta}\text{ (first level)} \tag{5.8}$$

Thus, the surface temperature $\overline{\theta}(z_s)$ is the mean of the values above and ”below” the surface.

The last term in Equation (6.4) denotes the anthropogenic head sources which are set to zero.

5.1.3 Humidity

The humidity at the surface can be kept constant or is calculated from a budget equation following Deardorff (1978):

$$\begin{aligned} \overline{q}^1_{1s} &= \alpha_q \overline{q}^1_{1sat}(\overline{T}_s) + (1-\alpha_q)\overline{q}^1_1 \quad \text{(first level)} \\ \overline{q}^1_{1s} &\leq \overline{q}^1_{1sat}(\overline{T}_s) \end{aligned} \tag{5.9}$$

The bulk soil water availability, α_q, can lie between W_s/W_k and 1 (α_q = Min (1, W_s/W_k). W_s denotes the bulk soil moisture content (depth of liquid water) down to the depth d_2 and W_k is the field capacity or saturated value of W_s given for each surface characteristic (values are provided in Appendix A.1). For α_q a prognostic equation is used:

$$\frac{\partial \alpha_q}{\partial t} = \frac{Q_E/l_{21} + P}{\rho_w W_k} \tag{5.10}$$

Q_E is calculated from the turbulent humidity flux $Q_E = l_{21}\rho_s q_* u_*$ (Section 3.3.1 for parameter averaging, Section 3.3.2 for flux averaging), P denotes the precipitation and ρ_w the density of water (value of 1000 kg/m^3 is used). Similar to equation (5.8), the humidity ‘below’ the surface is calculated from $\overline{q}^1_{1s}$ and $\overline{q}^1_1$ (first level).

5.1.4 Liquid Water

Liquid water is assumed to be deposed at the ground only in form of rain. From this assumption a zero flux boundary condition for the cloud water content arises, resulting in:

$$\overline{q}^{2c}_{1s} = \overline{q}^{2c}_1 \quad \text{(first level)} \tag{5.11}$$

The flux of rain water to the ground is equal to the flux at the first grid level:

$$\overline{w'q'^{2r}_1}\Big|_{z_s} = -V_{TR}\,\overline{q}^{2r}_1(z_1) \tag{5.12}$$

5.1.5 Pollutants

Pollutants are partly absorpted by vegetation, soil and water. At the topography height it can be written:

$$\frac{\partial \tilde{C}_j(z_s)}{\partial z} \neq 0 \quad \text{and} \quad \tilde{C}_j(z_s) \neq 0 \tag{5.13}$$

The partial absorption results from the concentration flux to the surface and depends on the deposition velocity v_d and the concentration $\overline{C}_j$ at the first grid level in height z_1:

$$\overline{w'C'_j} = -v_d\,\overline{C}_j(z_1) \tag{5.14}$$

The deposition velocity v_d depends on the turbulence in the atmosphere, chemical properties of the species, surface characteristics, and vegetation. Thus, no fixed value of v_d for all species and meteorological conditions can be given. In METRAS PC the deposition velocity can be calculated for 19 species.

The calculation of the deposition velocity V_D ist based on a resistance model, which means that V_D is calculated as a reciprocal value of the sum of three characteristic resistances (e.g. Chang et al., 1987):

$$V_D = (r_a + r_m + r_s)^{-1} \tag{5.15}$$

The intensity of turbulent mixing in the surface layer controls the aerodynamic resistance r_a. The following parameterization, used for instance also by Sheih et al. (1979), has been employed:

$$r_a = (u_*\kappa)^{-1} \cdot \left[ln\left(\frac{z_1}{z_0}\right) - \psi_h \right] \tag{5.16}$$

Here it is assumed that the turbulent transport of pollutants is similar to the transport of heat in the surface layer (e.g. Pielke, 1984) and the stability function ψ_h is calculated according to Dyer (1974) as given in Section 3.3, but taken as $\psi_h = 0$ for $-0.01 \leq z/L \leq 0.01$.

For parameterization of the sublayer resistance r_m different formulae are used for the 10 different land-use types considered in the model. Over a water surface the formulae discussed by Brutsaert (1975) and Garrat and Hicks (1973) are used:

$$r_m = \begin{cases} (u_*)^{-1} \cdot (13.6 \cdot Sc^{2/3} - 13.5) & \text{for} \quad Re < 1 \qquad (a) \\ (u_* \cdot \kappa)^{-1} \cdot \ln\left[\frac{u_*\kappa z_0}{D_c}\right] & \text{for} \quad Re \geq 1 \qquad (b) \end{cases} \tag{5.17}$$

with D_c the molecular diffusivity of the trace gas in air, $Sc = \nu / D_c$ the Schmidt number and Re the turbulent Reynolds number. Due to investigations performed by Garrat and Hicks (1973) r_m is calculated over vegetation by (Wesely and Hicks, 1977):

$$r_m = (u_* \kappa)^{-1} \cdot 2 \cdot Sc^{2/3} \tag{5.18}$$

For urban land use characteristics the formula pointed out by Brutsaert (1975) is applied:

$$r_m = u_*^{-1} \cdot (7.3 \cdot Re^{1/4} \cdot Sc^{1/2} - 5) \tag{5.19}$$

The surface resistance r_s depends on the stomata, cuticular and mesophyll resistances, and on the solubility or reactivity of a given trace gas (Walcek et al., 1986). For surfaces covered by vegetation the surface resistance is a function of season and insolation, and their influence on the stomata activity of the vegetation. Following Arrit et al. (1988), r_s is assumed to depend on the land-use type. The influence of insulation and relative humidity at the surface q_{rs} on the surface resistance r_s is included in the following way (Schlünzen and Pahl, 1992):

$$r_s = \begin{cases} r_{s,wet} & \text{for} \quad q_{rs} > 99.9\% & & (a) \\ r_{s,max} & \text{for} \quad q_{rs} < 99.9\% & \text{and} \quad R_{SW} = 0 \frac{W}{m^2} & (b) \\ r_{s,min} + (r_{s,max} - r_{s,min}) & \text{for} \quad q_{rs} < 99.9\% & \text{and} \quad 0 < R_{SW} < 400 \frac{W}{m^2} & \\ \quad \cdot [1 - (R_{SW}/400)^{1/3}] & & & (c) \\ r_{s,min} & \text{for} \quad q_{rs} < 99.9\% & \text{and} \quad R_{SW} \geq 400 \frac{W}{m^2} & (d) \end{cases} \tag{5.20}$$

The solar irradiation R_{SW} is calculated in the model METRAS PC as described in Section 3.7. For the values of $r_{s,wet}, r_{s,min}$, and $r_{s,max}$ used in METRAS PC see Appendix A.3.

In METRAS PC the concept of the resistance model is also applied to some aerosols (SO_4^{2-}, NO_3^-, Pb). The surface resistance r_s for aerosols smaller than 10 μm is about zero, the deposition only depends on the moleculare resistance and the size of the aerosols. For aerosols larger than 0.2 μm the deposition velocity increases with increasing diameter of the particle.

SO_4^{2-} and NO_3^- ions are mostly transported on other, larger particles. The mass size of the particles bearing SO_4^{2-} or NO_3^- varies with source, season, region and humidity. In general, SO_4^{2-} is dispersed in the $0.1 - 1.0 \mu m$ diameter range and nitrates are bimodally dispersed with one mode in the $0.1 - 1.0 \mu m$ range and the other in the $2.0 - 10.0 \mu m$ range (Voldner et al., 1986). Since large particles have higher deposition velocities, r_b for NO_3^- is more or less arbitrarily chosen to 50% of that for SO_4^{2-}. The time dependency of r_b for aerosols is solved in the same way as r_s for gaseous substances.

5.1.6 Subgrid Scale Fluxes

The turbulent momentum fluxes at the ground follow the boundary condition (Clark, 1977):

$$\tau_{11} = \tau_{22} = \tau_{33} = \tau_{12} = 0 \tag{5.21}$$

The stress tensor components $\tau_{13} = -\rho_o \overline{u'w'}$ and $\tau_{23} = -\rho_o \overline{v'w'}$ are derived from similarity theory. If the wind direction is given by $\alpha_d = \arctan(\bar{u}/\bar{v})$[1], τ_{13} and τ_{23} can be written

$$\begin{aligned} \tau_{13} &= \rho_0 u_*^2 \sin \alpha_d & (a) \\ \tau_{23} &= \rho_0 u_*^2 \cos \alpha_d & (b) \end{aligned} \tag{5.22}$$

With the parameter or flux averaging method given in Section 3.3.1 or 3.3.2 the momentum exchange between surface and atmosphere is completely described.

The horizontal turbulent fluxes of scalar variables at the ground follow the boundary condition (Clark, 1977):

$$\rho_0 \overline{u'\chi'} = \rho_0 \overline{v'\chi'} = 0 \quad ; \quad \chi = \theta, q, C_j \tag{5.23}$$

The vertical fluxes of scalar variables at the ground are derived from

$$\rho_0 \overline{w'\chi'} = -\rho_0 u_* \chi_* \quad ; \quad \chi = \theta, q \tag{5.24}$$

where the scaling variable χ_* is calculated by the parameter or flux averaging method given in Section 3.3.1 or 3.3.2 for temperature $\overline{\theta}$ and humidity $\overline{q_1^1}$. For concentrations Equation (5.14) is applied.

5.2 Upper Boundary

The upper model boundary is located at a height z_t (see Figure 2.1). Since no physical boundary exists in the atmosphere, the boundary conditions of the model must permit vertical propagating waves to leave the model area without reflections. It is assumed that the gradients of the horizontal wind components normal to the boundary vanish:

$$\begin{aligned} \left.\frac{\partial \bar{u}}{\partial z}\right|_{z_t} &= 0 & (a) \\ \left.\frac{\partial \bar{v}}{\partial z}\right|_{z_t} &= 0 & (b) \end{aligned} \tag{5.25}$$

[1]The wind direction is calculated in the model with the FORTRAN-function ATAN2, which has a continuous solution.

The vertical wind component also vanishes at the upper boundary:

$$\bar{w}|_{z_t} = 0 \tag{5.26}$$

From these assumptions it follows that the normal pressure gradient is also zero, $\partial\hat{p}_2/\partial\dot{x}^3 = 0$. To avoid reflections of vertically propagating waves at this rigid lid, absorbing layers are used in METRAS PC. They are realized by adding so–called Rayleigh damping terms to the model equations (2.22a—2.22c) and (2.26) to (2.28) (see Clark, 1977; Durran, 1981). These additional terms cause an increasing adaption of the prognostic variables to their corresponding and prescribed synoptic values with increasing height. In the equations of motion the damping terms are written:

$$\begin{aligned} R_1 &= -\rho_0 \overset{*}{\alpha} (\bar{u} - U_g)\, \nu_R && (a) \\ R_2 &= -\rho_0 \overset{*}{\alpha} (\bar{v} - V_g)\, \nu_R && (b) \\ R_3 &= -\rho_0 \overset{*}{\alpha}\, \bar{w}\, \nu_R && (c) \end{aligned} \tag{5.27}$$

The relaxation coefficient $\nu_R[s^{-1}]$ increases with height

$$\nu_R = \begin{cases} 0 & \text{for } k < k_D \\ \delta^{(k_t - k)} & \text{for } k \geq k_D \end{cases} \tag{5.28}$$

In Equation (5.28) k denotes the vertical grid point index, k_t the index of the highest grid point at the upper boundary and k_D the index of the first absorbing layer. From several tests $\delta[s^{-1}] = 0.2$ seems to be a good choice and $k = 4$ is used.

The absorbing layers damp vertically propagating waves and prevent their reflection at the upper boundary. To preserve the height of the area of interest the model area needs to be extended by the absorbing layers. Even though they are only implemented within the upper 4 layers they may influence the model result due to nonlinear interactions down to level $k_t - 8$. Thus the model area of interest should be increased by 8 levels. Alternative boundary conditions, e.g. to obtain the pressure field from a Fourier transformation of the vertical wind field (Klemp and Durran, 1983; Bougeault, 1983) are not implemented due to the low additional memory resources necessary for the absorbing layers and since these conditions might need smaller time steps for the model integration.

The temperature gradient at the model top results from the assumption $\overline{w'\theta'}|_{z_t} = 0$:

$$\left.\frac{\partial\bar{\theta}}{\partial z}\right|_{z_t} = 0 \tag{5.29}$$

The humidity, liquid water and concentration values are calculated from analogous boundary conditions. For pressure p_1 the value at the model top should be zero (Section 5.3.3). This results in the following equation:

$$p_1(\text{uppermost level}) = -p_1(\text{first level below model top}) \tag{5.30}$$

Consistent with the boundary conditions for velocities (5.21), the turbulent momentum fluxes and their gradients at the upper boundary are zero:

$$\begin{aligned} \tau_{13} &= \tau_{23} = \tau_{33} = 0 && (a) \\ \frac{\partial \tau_{11}}{\partial \dot{x}^3} &= \frac{\partial \tau_{22}}{\partial \dot{x}^3} = \frac{\partial \tau_{12}}{\partial \dot{x}^3} = 0 && (b) \end{aligned} \tag{5.31}$$

5.3 Lateral Boundaries

As the upper boundary, the lateral boundaries are artificial. On the one hand the lateral boundary conditions have to permit waves to leave the model area without reflections, on the other hand the synoptic values should influence the prognostic model variables at the inflow boundaries. The open boundary conditions are implemented in METRAS PC.

The robust non–reflecting boundary condition implemented in METRAS PC directly calculates the boundary normal wind components as far as possible from the prognostic equations. The boundary normal advection is treated by using the Orlanski (1976) condition at inflow boundaries and the upstream scheme at outflow boundaries. For the boundary parallel components of the velocity a zero–flux condition is assumed.

The boundary conditions used for momentum have to be considered in the formulation of the pressure boundary condition. For the pressure p_2 it follows that its gradient normal to the boundary vanishes. The normal gradients of temperature, humidity and concentrations usually are also set zero. For pressure p_1 no boundary values need to be specified but p_1 can be directly calculated from Equation (2.18).

Chapter 6

Initialization of the Model

The initialization of the three–dimensional model is done in three steps (see Figure 6.1). First, the spatial resolution of the model area and the location of the grid points have to be determined and the characteristic parameters of topography and land–use have to be interpolated to the grid points. In a second step a stationary data set is calculated by using the one–dimensional model version. This solution is used for initializing the three–dimensional model. During the initialization phase of the three–dimensional model the orography slowly grows (diastrophism) until the real orography heights have been established. The orography growing should take 10 min to 60 min dependent on the maximum topography height. As a rule of thumb the time for orography growing t_{maf} can be determined by

$$t_{maf} = \frac{z_{s,max}[m]}{0.1m/s} \tag{6.1}$$

In the following initialization phase the increased model accuracy should be continued. As a rule of thumb the time should be specified by

$$t_{mini} = 2t_{maf} \tag{6.2}$$

After a model integration time of altogether 2 to 8 hours (dependent in topography height and stratification) the model results are independent of the actual initialization phase. For pollution transport, however, the integration time might be longer before a stationary solution is achieved.

6.1 Initialization of Topography

The characteristic parameters orography height and land–use category are calculated for the grid points by use of the pre–processor GRITOP (Bigalke und Schlünzen, 2001). This pre–processor uses an area–weighting interpolation procedure and supplies the mesoscale

Determination of model area characteristics • Determination of grid representation • Interpolation of orography and land–use characteristics to grid points • Output of model area characteristics
Calculation of initial values (one–dimensional model) • Read of model area characteristics • Calculation of transformation coefficients • Read and calculation of consistent large–scale values • Read and calculation of consistent initial mesoscale values • Calculation of a stationary solution by numerical integration of the one-dimensional model equations
Calculation of initial values (three–dimensional model) • Read of model area characteristics • Calculation of transformation coefficients • Read of the one–dimensional stationary model result for the initialization grid point • Diastrophism and calculation of adapted large–scale and mesoscale values • Calculation of stationary or instationary solutions by numerical integration of the three–dimensional model equations (see Figure 4.1)

Figure 6.1: Initialization of the three–dimensional model (schematic description.)

model with information on the partial land—use. The characteristic parameters per land use characteristics are specified in the model (Appendix A.1).

6.2 Initialization of 1–d Model

From the area characteristic parameters the transformation coefficients are calculated at each grid point. After determining the topography height z_s for each grid point and the height of grid levels above flat terrain, the height of each grid point above the topography is calculated. Afterwards the large–scale and meso–scale values are read and interpolated to the model grid from the input values. Finally the one–dimensional model equations are integrated until the calculated meteorological profiles become stationary.

6.2.1 Large–Scale Values

For determining the geostrophic wind $\mathbf{V}_g$, potential temperature θ_o, specific humidity $q^1_{1\,o}$ and liquid water content $q^2_{1\,o}$, the following values have to be predefined:

- initialization grid point,
- pressure p_o at sea level,
- geostrophic wind $\mathbf{V}_g$ for the height of the initialization grid point or a profile of $\mathbf{V}_g$,
- temperature T_o for the height of the initialization grid point and a temperature gradient $\gamma = \partial T_o/\partial z$, or
- temperature profile T_o starting from the height of the initialization grid point,
- profile of the relative humidity,
- profile of liquid water content $q^2_{1\,o}$,
- values for the temperature in the soil and in water $T(-h_\theta)$.

Note that the pressure value is sea level pressure while all other values are given for heights above initialization grid point. Therefore, when using profile information for e.g. temperature, the lowest height is 0 m. The initial data need to be given in accordance with the application under consideration. They are taken from observations, weather charts or analysis (e.g. Luthardt, 1987). For the calculation of consistent large–scale values the hydrostatic (2.16) and geostrophic approximation (2.17) are presumed in the model. Assuming a constant temperature gradient within each grid layer the temperature profile follows from:

$$T_o(z) = T_o(NN) + \gamma \cdot z \tag{6.3}$$

The hydrostatic assumption together with the layer-wise constant temperature gradient γ yields the pressure profile

$$p_o(z) = p_o(NN)\left(\frac{T_o(z)}{T_o(NN)}\right)^{-g/(R\cdot\gamma)} \tag{6.4}$$

The density ρ_o is calculated by use of the ideal gas law as a function of pressure and temperature:

$$\rho_o = \frac{p_o}{RT_o} \tag{6.5}$$

If not predefined, the potential temperature θ_o can be derived from the large-scale profiles by use of (2.5).

6.2.2 Mesoscale Values

Due to the assumption of horizontal homogenity no vertical winds can develop in the one–dimensional model version. Thus the vertical wind component $\hat{w}$ and the mesoscale pressure p_2 are zero, resulting in $\tilde{p} = p_1$ for the one–dimensional case. Usually, the initial temperature pertubation $\tilde{T}$ is zero, too, but it can also be prescribed by a measured temperature profile. The mesoscale density deviation $\tilde{\rho}$ is calculated by (2.19) and the mesoscale pressure p_1 by (2.18). Now the mesoscale density $\tilde{\rho}$ can be calculated again. This iteration procedure is continued until the changes in $\tilde{\rho}$ become very small, namely $| \Delta\tilde{\rho} | < 0.01 \cdot | \tilde{\rho} |$. Now the potential temperature $\tilde{\theta}$ can be calculated by:

$$\tilde{\theta} = \tilde{T} \left(\frac{P_r}{p_o + \tilde{p}} \right)^{R/c_p} - \theta_o \left\{ 1 - \left(\frac{p_o}{p_o + \tilde{p}} \right)^{R/c_p} \right\} \tag{6.6}$$

The horizontal wind components are initialized by using the values of the geostrophic components. Due to the integration of the one–dimensional model the Coriolis effects and vertical exchange are considered in the model and should not be included in the input data. If friction and veering of the wind is already part of the initial data, resulting wind speeds are too low and the wind direction is wrong, too.

6.2.3 Stationarity

The one–dimensional model equations are integrated starting with the pre–defined initial profiles and using the same boundary conditions but without diurnal cycle as in the three–dimensional model. When starting the integration the wind profiles are not adapted to the thermodynamic variables and reverse. Thus the dynamic equations are integrated with a fixed temperature profile until the wind profiles become stationary. Stationarity is defined by

$$|\Delta\psi| \;<\; a \cdot \Delta t \tag{6.7}$$

where ψ stands for the horizontal wind components $\overline{u}$ or $\overline{v}$ and $\Delta\psi$ denotes changes of ψ from one time step to the next. The constant a is derived from a scale analysis of the equation of motion for typical mesoscale phenomena: In the one-dimensional model equations the Coriolis force with an acceleration $f\bar{u}$ is small compared to the other forces. For mean latitudes with $f \simeq 10^{-4}[s^{-1}], |\bar{u}| \simeq 10[m/s]$ the acceleration results in $f\overline{u} \simeq 10^{-3}[m/s^2]$. Stationarity is assumed, if changes of $\overline{u}$ and $\overline{v}$ during one time step are less than 1 % of the maximum Coriolis acceleration. From this a value of $a = 10^{-5}[m/s^2]$ can be derived for the one-dimensional model version. For a sufficient damping of inertial oszillations the simulations should be done for several days. Usually a simulation is interrupted after 80.000 time steps even if the profiles are not stationary.

After the wind profiles are stationary, wind and temperature are integrated simultaneously until all profiles are stationary again. These profiles are transfered to the three-dimensional model for initialization.

6.3 Initialization of 3–d Model

From the one–dimensional model the transformation coefficients are taken. All the topography heights above or below the altitude of the initialization grid point are neglected at first and the stationary profiles of the one–dimensional model are expanded over the model area assuming horizontal homogenity. Afterwards the initialization by diastrophism (see Groß, 1984) starts. This means that the surface heights grow or shrink from time step to time step until the real heights are achieved. During the process of diastrophism the vertical coordinate η (Equation 2.6) changes according to

$$z_{s,p}^{n+1} = z_{s,p}^{n} + A_f \cdot z_s \tag{6.8}$$

z_s denotes the final surface height, A_f the reziproce of the time (t_{maf}) or the number of time steps for diastrophism, and $z_{s,p}^n$ the temporal surface height at time $n \cdot \Delta t$. $1/A_f$ typically lies between 100 and 1000 and should ensure that vertical winds arising from the topography growing do not exceed 0.1 m/s (Equation 6.1). The artificial vertical winds caused by the diastrophy decrease with increasing integration time.

The large–scale values are adapted to the actual topography heights at each time step. They remain horizontal homogenous with respect to sea level. As an example the adaption of the large–scale temperature follows:

$$T_0^n(x,y,z) = T_0(NN) + \gamma \left(z \frac{z_t - z_{s,p}^n(x,y)}{z_t} + z_{s,p}^n(x,y) \right) \tag{6.9}$$

The large–scale pressure p_0 and density ρ_0 are calculated from (6.4) and (6.5), respectively, and the potential temperature from (2.5).

In contrast to the large–scale values the mesoscale variables are adapted to the changing coordinate system by integrating the prognostic equations for $1/A_f$ time steps. The integration is continued without interruption if not otherwise specified by the user. It is usually assumed that the meteorological fields are independent from initialization phase after about three hours of integration time. For unstable stratification the initialization time might take up to 8 hours.

Chapter 7

Validation

METRAS PC is based on the model METRAS and has mostly the same characteristics. With the model METRAS PC qualities the following applications where performed with METRAS:

A sea breeze studies (Schlünzen, 1988, 1990; Wu and Schlünzen, 1992; Schlünzen and Pahl, 1992; Scheng et al., 2000; Schrum et al., 1997),

B passive tracer transport (Bigalke, 1992; Schlünzen and Pahl, 1992; Schlünzen and Krell, 1994; Beddig et al., 1997; Schlünzen et al., 1997),

C steep terrain influences (Niemeier and Schlünzen, 1996; von Salzen et al., 1996; Scheng et al., 2000),

D A model evaluation scheme was developed (Schlünzen, 1996, 1997) and applied to METRAS (Dierer, 1998).

E boundary layer development (Lüpkes, Schlünzen, 1996; von Salzen et al., 1996).

METRAS PC is validated by using the test cases specified in the EVA program of METRAS+.

Appendix A

Mathematical Hints

A.1 Parameters for the Different Land Use Categories

Type	Class j	A_0	k_s $[m^2 s^{-1}]$	ν_s $[J(Ksm)^{-1}]$	$[m]$	W_k α_q	z_0 $[m]$
Water	0	$f(Z(t))$	$0.15 \cdot 10^{-6}$	100.0	0.98	100.0	$f(u_*)$
Mudflats	1	0.10	$0.74 \cdot 10^{-6}$	2.20	0.98	0.322	0.0004
Sand	2	0.20	$0.57 \cdot 10^{-6}$	1.05	0.10	0.026	0.0012
Mixed land use	3	0.20	$0.52 \cdot 10^{-6}$	1.33	0.20	0.138	0.04
Meadows	4	0.20	$0.52 \cdot 10^{-6}$	1.33	0.40	0.015	0.02
Heath	5	0.15	$0.24 \cdot 10^{-6}$	0.30	0.10	0.423	0.05
Bushes	6	0.20	$0.52 \cdot 10^{-6}$	1.33	0.30	0.081	0.10
Mixed forest	7	0.15	$0.80 \cdot 10^{-6}$	2.16	0.30	0.121	1.00
Coniferous forest	8	0.10	$0.80 \cdot 10^{-6}$	2.16	0.30	0.161	1.20
Urban area	9	0.15	$1.40 \cdot 10^{-6}$	2.93	0.05	0.968	0.70

Table A.1: Surface characteristics (Albedo A, thermal diffusivity k_s, thermal conductivity ν_s, soil water availability α (start value), saturation value for water content W_k, roughness length z_o) for the 10 surface types, typically used in METRAS.

A.2 Calculation of Zenit Angle and Incoming Solar Radiation

The incoming solar radiation is calculated with respect to

- geographical location of the model grid point,
- date and time of the model run,
- surface slope,
- shading of areas due to neighbouring hills etc. and
- rotation of the used coordinate system with respect to north.

The following derivation is given by Iqbal (1983). For the meaning of symbols within this section see the symbol table at the end of this appendix.

For a given geographic latitude φ, in the absence of the earth's refractive atmosphere, the trigonometric relation between the sun and a horizontal surface is (Sellers, 1974)

$$\cos Z(t) = \sin\delta \;\sin\varphi + \cos\delta \;\cos\varphi \;\cos w = \sin \;\alpha \tag{A.1}$$

where the declination δ is given by

$$\begin{aligned}\delta \;=\; & 0.006918 - 0.399912\cos(d_o) + 0.070257\sin(d_o) \\ & -0.006758\cos(2d_o) + 0.000907\sin(2d_o) \\ & -0.002697\cos(3d_o) + 0.001480\sin(3d_o)\end{aligned} \tag{A.2}$$

This equation gives the declination in radians (Pielke, 1984, p. 225). d_o is the Julian day. The hour angle w is defined by

$$w = 180^o - s \cdot \frac{15^o}{3600} \tag{A.3}$$

with s seconds since midnight. $\cos Z(t)$ has to be restricted to values between 0 and 1.

For inclined surfaces it is necessary to prescribe the slope of the surface with respect to the horizontal position and its orientation in relation to the local meridian. The inclination of a surface from the horizontal position can be caluclated by

$$\beta = \arctan\left(\sqrt{\left(\frac{\Delta z_x}{\Delta x}\right)^2 + \left(\frac{\Delta z_y}{\Delta y}\right)^2}\right) \tag{A.4}$$

where Δz_x is the difference in surface height with respect to the x–direction, Δz_y analogous for the y–direction. From the known values for the surface's inclination, β, orientation of the slope γ and solar azimuth ψ the angle θ between the normal to the surface and sun–earth vector is given by

$$\cos\theta \quad = \quad \cos\beta\ \cos Z(t) + \sin\beta\ \sin z(t)\ \cos(\psi - \gamma) \tag{A.5}$$

The solar azimuth ψ can be taken from

$$\cos\psi \quad = \quad \frac{\sin(90° - Z(t))\sin\varphi - \sin\delta}{\cos(90° - Z(t))\cos\varphi} \tag{A.6}$$

and then

$$\psi \quad = \quad \arccos(\cos\psi) \cdot sign\ (w) \tag{A.7}$$

to ensure the right sign of ψ due to its definition (see symbol table). For the determination of γ with respect to south direction a possibly given rotation angle ξ of the used coordinate system has to be taken into account. γ is calculated by means of the FORTRAN standard function ATAN2:

$$\gamma \quad = \quad -\text{ATAN2}\left(\cos\xi \cdot \frac{\Delta z}{\Delta x} - \sin\xi \cdot \frac{\Delta z}{\Delta y},\ \sin\xi \cdot \frac{\Delta z}{\Delta x} + \cos\xi \cdot \frac{\Delta z}{\Delta y}\right) \tag{A.8}$$

Each grid point of the model area can be shaded by the topography given at other grid points, if the solar altitude is lower than the altitude of the topography in the direction of the solar azimuth. For taking these shading effects into account twelve azimuth sectors are defined at each grid point. Sector 1 is defined by $+180° \geq \psi_m > +165°$, sector 2 by $+165° \geq \psi_m > +135°$ and so on by steps of 30° where $\pm 180°$ corresponds to north direction. The sector with $-165° \geq \psi_m \geq 180°$ belongs to sector 1 again. Considering the possible rotation of the coordinate system, ψ_m is also calculated by means of the FORTRAN function ATAN2:

$$\psi_m \quad = \quad \text{ATAN2}\ (\cos\xi\ \Delta x - \sin\xi\ \Delta y, -\sin\xi\ \Delta x - \cos\xi\ \Delta y) \tag{A.9}$$

When starting the model run a minimum solar altitude α_m is calculated at each grid point and for each sector by

$$\alpha_m \quad = \quad \max\left(\arctan\left(\frac{\Delta z}{\Delta s}\right)\ , \varphi\right) \tag{A.10}$$

which defines a minimum solar altitude for the corresponding azimuth sector (Figure A.1). Δz is the difference in topography height between this grid point and any other grid point within the selected azimuth sector, Δs is the horizontal distance between both grid points. If the solar azimuth ψ belongs to an azimuth sector ψ_m a grid point is shaded as long as the solar altitude α is lower than the corresponding minimum solar altitude $\alpha_m = f(\psi_m, x, y)$.

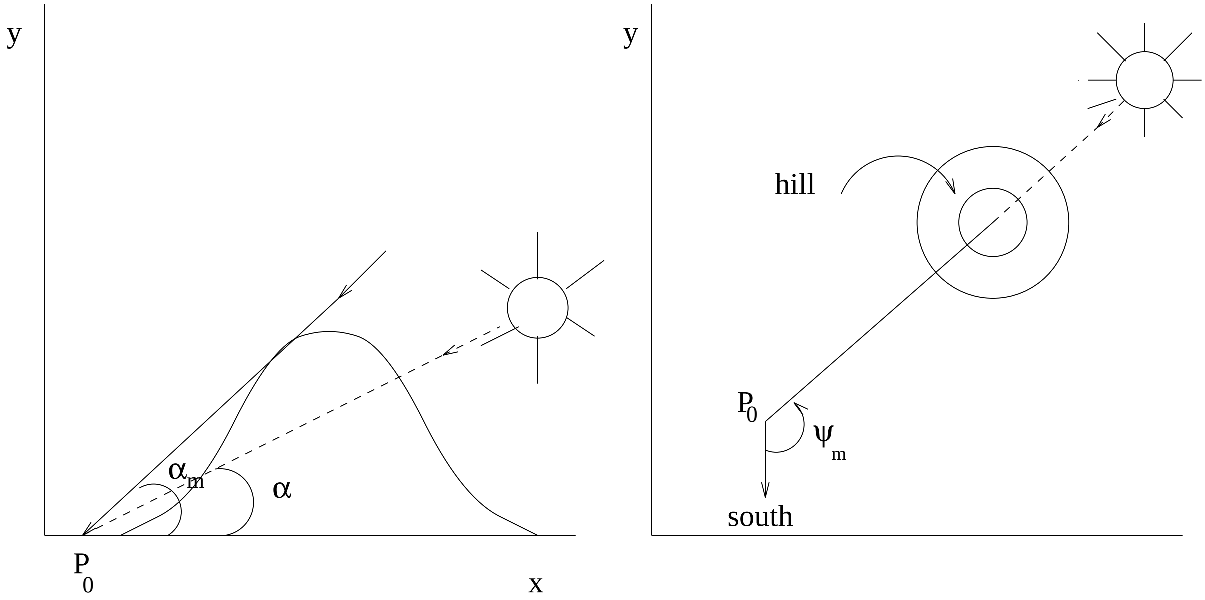

Figure A.1: Definition of azimuth ψ_m and minimum solar altitude α_m at grid point P_o.

Symbol Table for Appendix A.2

symbol	**name**	**values**	**meaning/comments**
α	solar altitude	$0° \leq \alpha \leq 90°$	angular elevation of the sun above the true horizon (degrees)
β	surface inclination	$0° \leq \beta \leq 90°$	inclination of a surface from the horizontal position (degrees)
γ	surface azimuth	$-180° \leq \gamma \leq +180°$	surface azimuth angle, that is, the deviation of the normal to the surface with respect to the local meridian, south zero, east positive (degrees)
δ	declination	$-23.5° \leq \delta \leq +23.5°$	angular position of the sun at solar noon with respect to the plane of the equator, north positive (degrees)
θ	suns angle to inclinated surface	$0° \leq \theta \leq 90°$	angle of incidence for an arbitrary oriented surface, the angle between normal to the surface and sun–earth vector (degrees)
$Z(t)$	zenith angle	$0° \leq Z(t) \leq 90°$	angular position of sun with respect to the local vertical, $\theta_z = 90° - \alpha$ (degrees)
φ	latitude	$-90° \leq \varphi \leq +90°$	geographic latitude, north positive (degrees)
ψ	azimuth	$-180° \leq \psi \leq +180°$	solar azimuth, south zero, east positive (degrees)
w	hour angle	$-180° \leq w \leq +180°$	solar noon zero and morning positive (degrees); changes 15° every hour (e.g. $w = +15°$ at 11:00 and $w = -37.5°$ at 14:30)
ξ	rotation angle	$0° \leq \xi \leq 360°$	rotation of model's coordinate system against north (e.g. $\xi = 0°$ with x–axis to east, and $\xi = 135°$ with x–axis to north–west)

A.3 Surface Resistance Values

land-use type	season	resistance parameters $r_{s,min}$ $[s/m]$	$r_{s,max}$ $[s/m]$	$r_{s,wet}$ $[s/m]$	variable name in METRAS
water	spring	0	0	0	DEPRO
	summer	0	0	0	DEPRO
	early autumn	0	0	0	DEPRO
	late autumn	0	0	0	DEPRO
	winter	0	0	0	DEPRO
mudflat	spring	100	100	100	DEPOS
	summer	100	100	100	DEPOS
	early autumn	100	100	100	DEPOS
	late autumn	100	100	100	DEPOS
	winter	100	100	100	DEPOS
sand	spring	1000	1000	1000	DEPOS
	summer	1000	1000	1000	DEPOS
	early autumn	1000	1000	1000	DEPOS
	late autumn	1000	1000	1000	DEPOS
	winter	1000	1000	1000	DEPOS
mixed vegetation	spring	50	100	0	DEPOS
	summer	70	500	0	DEPOS
	early autumn	500	500	100	DEPOS
	late autumn	50	50	50	DEPOS
	winter	100	100	100	DEPOS
wet grass	spring	100	400	0	DEPOS
	summer	100	500	0	DEPOS
	early autumn	500	500	100	DEPOS
	late autumn	500	500	100	DEPOS
	winter	100	100	100	DEPOS
heath	spring	75	250	0	DEPOS
	summer	100	500	0	DEPOS
	early autumn	500	500	100	DEPOS
	late autumn	200	200	100	DEPOS
	winter	100	100	100	DEPOS
bushes	spring	100	1000	0	DEPOS
	summer	70	1000	0	DEPOS
	early autumn	800	800	300	DEPOS
	late autumn	800	1000	300	DEPOS
	winter	800	800	800	DEPOS
mixed forest	spring	100	1000	0	DEPOS
	summer	60	1000	0	DEPOS
	early autumn	1000	1000	500	DEPOS
	late autumn	1000	1000	500	DEPOS
	winter	1000	1000	1000	DEPOS
coniferous forest	spring	150	1000	0	DEPOS
	summer	150	1000	0	DEPOS
	early autumn	800	800	100	DEPOS
	late autumn	800	1000	100	DEPOS
	winter	500	500	500	DEPOS
urban areas	spring	1000	1000	1000	DEPOS
	summer	1000	1000	0	DEPOS
	early autumn	1000	1000	1000	DEPOS
	late autumn	1000	1000	1000	DEPOS
	winter	200	200	200	DEPOS

Table A.2: Parameters $r_{s,min}, r_{s,max}$ and $r_{s,wet}$ for SO_2

land-use type	season	resistance parameters $r_{s,min}$ $[s/m]$	$r_{s,max}$ $[s/m]$	$r_{s,wet}$ $[s/m]$	variable name in METRAS
water	spring	0	0	0	DEPRO
	summer	0	0	0	DEPRO
	early autumn	0	0	0	DEPRO
	late autumn	0	0	0	DEPRO
	winter	0	0	0	DEPRO
mudflat	spring	300	400	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	200	400	0	DEPOS
	late autumn	300	400	0	DEPOS
	winter	1000	2500	0	DEPOS
sand	spring	600	1200	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	400	800	0	DEPOS
	late autumn	600	1200	0	DEPOS
	winter	2000	4000	0	DEPOS
mixed vegetation	spring	500	1000	0	DEPOS
	summer	300	600	0	DEPOS
	early autumn	500	1000	0	DEPOS
	late autumn	500	1000	0	DEPOS
	winter	1000	2500	0	DEPOS
wet grass	spring	400	600	0	DEPOS
	summer	300	600	0	DEPOS
	early autumn	300	600	0	DEPOS
	late autumn	400	600	0	DEPOS
	winter	1000	2500	0	DEPOS
heath	spring	320	650	0	DEPOS
	summer	220	450	0	DEPOS
	early autumn	320	650	0	DEPOS
	late autumn	320	650	0	DEPOS
	winter	570	1400	0	DEPOS
bushes	spring	400	800	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	350	700	0	DEPOS
	late autumn	400	800	0	DEPOS
	winter	1000	2250	0	DEPOS
mixed forest	spring	300	600	0	DEPOS
	summer	100	200	0	DEPOS
	early autumn	200	400	0	DEPOS
	late autumn	300	600	0	DEPOS
	winter	1000	2000	0	DEPOS
coniferous forest	spring	140	300	0	DEPOS
	summer	140	300	0	DEPOS
	early autumn	140	300	0	DEPOS
	late autumn	140	300	0	DEPOS
	winter	140	300	0	DEPOS
urban areas	spring	600	1200	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	400	800	0	DEPOS
	late autumn	600	1200	0	DEPOS
	winter	2000	4000	0	DEPOS

Table A.3: Parameters $r_{s,min}$, $r_{s,max}$, and $r_{s,wet}$ for SO_4^{2-}.

land-use type	season	resistance parameters $r_{s,min}$ $[s/m]$	$r_{s,max}$ $[s/m]$	$r_{s,wet}$ $[s/m]$	variable name in METRAS
water	spring	0	0	0	DEPRO
	summer	0	0	0	DEPRO
	early autumn	0	0	0	DEPRO
	late autumn	0	0	0	DEPRO
	winter	0	0	0	DEPRO
mudflat	spring	300	400	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	200	400	0	DEPOS
	late autumn	300	400	0	DEPOS
	winter	1000	2500	0	DEPOS
sand	spring	600	1200	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	400	800	0	DEPOS
	late autumn	600	1200	0	DEPOS
	winter	2000	4000	0	DEPOS
mixed vegetation	spring	500	1000	0	DEPOS
	summer	300	600	0	DEPOS
	early autumn	500	1000	0	DEPOS
	late autumn	500	1000	0	DEPOS
	winter	1000	2500	0	DEPOS
wet grass	spring	400	600	0	DEPOS
	summer	300	600	0	DEPOS
	early autumn	300	600	0	DEPOS
	late autumn	400	600	0	DEPOS
	winter	1000	2500	0	DEPOS
heath	spring	320	650	0	DEPOS
	summer	220	450	0	DEPOS
	early autumn	320	650	0	DEPOS
	late autumn	320	650	0	DEPOS
	winter	570	1400	0	DEPOS
bushes	spring	400	800	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	350	700	0	DEPOS
	late autumn	400	800	0	DEPOS
	winter	1000	2550	0	DEPOS
mixed forest	spring	300	600	0	DEPOS
	summer	100	200	0	DEPOS
	early autumn	200	400	0	DEPOS
	late autumn	300	600	0	DEPOS
	winter	1000	2000	0	DEPOS
coniferous forest	spring	140	300	0	DEPOS
	summer	140	300	0	DEPOS
	early autumn	140	300	0	DEPOS
	late autumn	140	300	0	DEPOS
	winter	140	300	0	DEPOS
urban areas	spring	600	1200	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	400	800	0	DEPOS
	late autumn	600	1200	0	DEPOS
	winter	2000	4000	0	DEPOS

Table A.4: Parameters $r_{s,min}$, $r_{s,max}$, and $r_{s,wet}$ for NO_3^-.

land-use type	season	resistance parameters $r_{s,min}$ $[s/m]$	$r_{s,max}$ $[s/m]$	$r_{s,wet}$ $[s/m]$	variable name in METRAS
water	spring	0	0	0	DEPRO
	summer	0	0	0	DEPRO
	early autumn	0	0	0	DEPRO
	late autumn	0	0	0	DEPRO
	winter	0	0	0	DEPRO
mudflat	spring	300	400	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	200	400	0	DEPOS
	late autumn	300	400	0	DEPOS
	winter	1000	2500	0	DEPOS
sand	spring	600	1200	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	400	800	0	DEPOS
	late autumn	600	1200	0	DEPOS
	winter	2000	4000	0	DEPOS
mixed vegetation	spring	500	1000	0	DEPOS
	summer	300	600	0	DEPOS
	early autumn	500	1000	0	DEPOS
	late autumn	500	1000	0	DEPOS
	winter	1000	2500	0	DEPOS
wet grass	spring	400	600	0	DEPOS
	summer	300	600	0	DEPOS
	early autumn	300	600	0	DEPOS
	late autumn	400	600	0	DEPOS
	winter	1000	2500	0	DEPOS
heath	spring	320	650	0	DEPOS
	summer	220	450	0	DEPOS
	early autumn	320	650	0	DEPOS
	late autumn	320	650	0	DEPOS
	winter	570	1400	0	DEPOS
bushes	spring	400	800	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	350	700	0	DEPOS
	late autumn	400	800	0	DEPOS
	winter	1000	2250	0	DEPOS
mixed forest	spring	300	600	0	DEPOS
	summer	100	200	0	DEPOS
	early autumn	200	400	0	DEPOS
	late autumn	300	600	0	DEPOS
	winter	1000	2000	0	DEPOS
coniferous forest	spring	140	300	0	DEPOS
	summer	140	300	0	DEPOS
	early autumn	140	300	0	DEPOS
	late autumn	140	300	0	DEPOS
	winter	140	300	0	DEPOS
urban areas	spring	600	1200	0	DEPOS
	summer	200	400	0	DEPOS
	early autumn	400	800	0	DEPOS
	late autumn	600	1200	0	DEPOS
	winter	2000	4000	0	DEPOS

Table A.5: Parameters $r_{s,min}$, $r_{s,max}$, and $r_{s,wet}$ for *Pb*.

Appendix B

List of Symbols

A_f	control value for diastrophism
A_0	Albedo
a	stationarity parameter
C_j	pollutant concentration
C_{j*}	scaling value of concentration
c_p	specific heat of dry air at constant pressure
c_v	specific heat of dry air at constant volume
$\mathbf{F}$	moleculare friction
F	transformation coefficient
f	Coriolis parameter $(2\Omega sin\varphi)$
f'	Coriolis parameter $(2\Omega cos\varphi)$
g	gravity acceleration
$\dot{g}$	determinant $\lvert\dot{g}_{ij}\rvert$
$\dot{g}_{il}$	covariant metric tensor
$\dot{g}^{il}$	contravariant metric tensor
H_s	characteristic vertical scale of a phenomen
h_θ	depth of temperature wave
h	topography height
$\mathbf{i}$	unit vector in west-east direction

$\mathbf{j}$	unit vector in south-north direction
K_{hor}	horizontal exchange coefficient for momentum
$K_{hor,\chi}$	horizontal exchange coefficient for scalar quantities
K_{vert}	vertical exchange coefficient for momentum
$K_{vert,\chi}$	vertical exchange coefficient for scalar quantities
$\mathbf{k}$	unit vector in vertical direction
k_s	thermal diffusivity
L	Monin Obukhov length
L_S	characteristical horizontal scale of a phenomen
l_b	blending height
l_x	scale of horizontal extension of subgrid-scale surface elements
l_{21}	latent heat of vaporization of water
p	pressure
p_o	large-scale pressure
p_1	mesoscale "thermic" pressure
p_2	mesoscale "dynamic" pressure
$\tilde{p}$	mesoscale pressure
$\overline{p}$	mean pressure value
p'	pressure fluctuation
Q_χ	sources and sinks in the balance equation of scalar quantities χ
$\dot{\mathbf{q}}_i$	covariant basis vectors in coordinate system $\dot{X}$
$\dot{\mathbf{q}}^i$	contravariant basis vectors in coordinate system $\dot{X}$
q_1^1	specific humidity
$q_{1^s}^1$	surface humidity
$q_{1^{sat}}^1$	saturation value of surface humidity
$q_{0_i}^1$	large scale part of $q_i^1 (i = 1, 2, 3)$
$\tilde{q}_i^{\,1}$	meso-scale part of $q_i^1 (i = 1, 2, 3)$
$\hat{q}_i^{\,1}$	'temporal' value of $q_i^1 (i = 1, 2, 3)$

q_1^2 liquid water content [kg] per kg humid air (dry air and water)

q_1^3 ice content [kg] per kg air (dry air and ice)

q_* scaling value for specific humidity

q_*^j subgrid scale scaling value for specific humidity

R universal gas constant

R_o gas constant of dry air

R_1^1 gas constant of water vapour

R_i^k individual gas constant

R_i^* modified Richardson number

$\mathbf{r}$ location vector

r relative humidity

T temperature

T_o large-scale temperature

T_s surface temperature

t time

U_g geostrophic wind in west-east direction

u velocity in west-east-direction

$\hat{u}$ temporal velocity in west-east direction

u' velocity fluctuation in west-east direction

u_i velocity components in cartesian coordinates

$\bar{u}$ mean velocity in west-east direction

$\dot{u}_i$ covariant velocity component

$\dot{u}^i$ contravariant velocity component

$\overline{\dot{u}}^i$ mean contravariant velocity component

$\dot{u}^{i\prime}$ contravariant component of velocity fluctuation

u_* friction velocity

u_*^j subgrid scale friction velocity

V magnitude of horizontal wind

$\mathbf{V_g}$	geostrophic wind vector
V_g	geostrophic wind in south-north direction
V_{TR}	terminal velocity of rain drops
$\mathbf{v}$	velocity vector
v	velocity in south-north direction
$\hat{v}$	temporal velocity in south-north direction
v_d	deposition velocity
$\bar{v}$	mean velocity in south-north direction
v^k	specific volume
W_s	bulk moisture content
W_k	saturated value of W_s
w	vertical velocity
$\hat{w}$	temporal vertical velocity
$\bar{w}$	mean vertical velocity
X	Cartesian coordinate system
$\dot{X}$	terrain-following coordinate system
x	horizontal coordinate in west-east direction in coordinate system X
$\dot{x}^i$	coordinate in coordinate system $\dot{X}$
y	horizontal coordinate in south-north direction in coordinate system X
$Z(t)$	zenit angle
z	vertical coordinate in coordinate system X
z_s	topographic height in coordinate system X
z_t	height of model top
z_o	mean roughness length
z_o^j	subgrid-scale roughness length
α	ratio of exchange coefficients for scalar quantities and momentum
α_d	wind direction
$\overset{*}{\alpha}$	grid volume

β function for calculating changes in specific humidity

$\dot{\Gamma}^{i}{}_{j,k}$ Christoffel symbol

γ temperature gradient

Δt time step

Δx longitudinal grid increment

$\Delta \dot{x}^1$ grid increment in west-east direction in coordinate system $\dot{X}$

$\Delta \dot{x}^2$ grid increment in south-north direction in coordinate system $\dot{X}$

$\Delta \dot{x}^3$ vertical grid increment in coordinate system $\dot{X}$

Δy lateral grid increment

Δz vertical grid increment

ν kinematic viscosity of air

ν_R damping coefficient

ν_s thermal conductivity

η vertical coordinate in coordinate system $\dot{X}$

θ potential temperature

θ_o large-scale part of potential temperature

$\tilde{\theta}$ meso-scale part of potential temperature

θ' potential temperature fluctuation

θ_* scaling value of temperature

θ_*^j subgrid-scale scaling value of temperarure

$\tilde{\theta}_{Mean}$ area mean temperature values

$\hat{\theta}$ 'temporal' value of potential temperature

κ von Karman constant

ρ density of air

ρ_o large-scale part of density

$\tilde{\rho}$ meso-scale part of density

$\overline{\rho}$ mean density

ρ' density fluctuation

τ_{ij} component of turbulent stress tensor

Φ geopotential

φ geographic latitude

χ any scalar quantity

$\tilde{\chi}$ meso-scale part of scalar quantity χ

$\overline{\chi}$ mean value of scalar quantity χ

$\hat{\chi}$ 'temporal' value of scalar quantity χ

χ' fluctuation of scalar quantity χ

χ_0 large-scale part of scalar quantity χ

ψ any quantity

$\tilde{\psi}$ meso-scale part of ψ

$\overline{\psi}$ mean value of ψ

ψ' fluctuation of ψ

ψ_o large-scale part of ψ

ψ_m stability function of momentum

ψ_h stability function of heat

$\mathbf{\Omega}$ angular velocity vector of the earth

Ω magnitude of Ω

Ω_i covariant component of earth's angular velocity vector

∇ gradient operator

$\Box x$ area size in west-east direction

$\Box y$ area size in south-north direction

Appendix C

References

C.1 Additional Model Descriptions

For further information on the preprocessors of the model METRAS PC the following descriptions are available:

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C.2 References on Model METRAS and METRAS PC

An actual version of model references is available from the internet at [`http://www.mi.uni-hamburg.de/technische_meteorologie/Meso/metras/metras_publications.html`]. The developers of METRAS PC would very much appreciate to receive copies of publications made by using results of model METRAS PC.

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EVA (Version 1.0)

Ein Programm zur Evaluierung mesoskaliger Modelle gemäß VDI Richtlinie 3783, Blatt 7

Programmdokumentation

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1. Einführung

Die VDI Richtlinie 3783 Blatt 7 „Prognostische mesoskalige nichthydrostatische Windfeldmodelle – Evaluierung für dynamisch und thermisch bedingte Strömungsfelder“ [1] formuliert Anforderungskriterien zur Qualitätssicherung mesoskaliger Simulationsmodelle. Modelle, die diese Anforderungskriterien erfüllen, gelten als evaluiert im Sinne der Richtlinie. Der Evaluierungsprozess eines Modells, bezogen auf eine bestimmte Modellversion, ist in Form eines Evaluierungsprotokolls festzuhalten, das gegenüber Auftraggebern oder Behörden als Nachweis einer erfolgreichen Evaluierung verwendet werden kann.

Das Programm EVA ist eine programmtechnische Umsetzung der VDI Richtlinie und erleichtert die Realisierung des Evaluierungsprozesses für ein beliebiges mesoskaliges Modell. Der Anwender von EVA beantwortet über die Eingabesteuerung des Programms Fragen nach den notwendigen und optionalen Eigenschaften des Modells und seiner Anwendung und stellt Modellergebnisdateien zu den insgesamt sieben in der Richtlinie definierten Testfällen bereit. EVA kontrolliert die notwendigen Modelleigenschaften, berechnet Trefferquoten des Modells für die Testfälle und erstellt ein „Evaluierungszertifikat“ (Evaluierungsprotokoll), das vom Anwender ausgedruckt und unterschrieben als Evaluierungsnachweis verwendet werden kann.

Dem Anwender des Modells METRAS PC [2] bietet EVA den Vorteil, dass Modellergebnisdateien von METRAS PC ohne vorherige Konvertierung direkt dem Evaluierungsprogramm bereitgestellt werden können. EVA konvertiert METRAS PC Ergebnisdateien automatisch in das vorgeschriebene Format.

EVA 1.0 liegt als Einzelversion und als eine in das Programmsystem **METRAS$^+$** (Version 1.0) [3] integrierte Programmversion vor. Diese Dokumentation bezieht sich auf beide Programmversionen. Abschnitte, die für **METRAS$^+$** irrelevant sind, sind gesondert gekennzeichnet.

2. Anforderungskriterien der Richtlinie

Die Evaluierungsrichtlinie VDI 3783, Blatt 7 schreibt nicht ein bestimmtes Modell oder feste Modelleigenschaften vor, sondern formuliert Mindestanforderungen an Modelle und Vorschriften zur Evaluierung. Im Folgenden wird das grundlegende Konzept der Richtlinie zusammengefasst. Die Einzelheiten sind dem Richtlinientext [1] zu entnehmen. Sie werden im weiteren Verlauf dieser Dokumentation nur soweit erläutert[3], wie es zum Verständnis des Programms notwendig ist.

Die Anforderungen der VDI-Richtlinie an Modelle gliedern sich in drei Bereiche.

2.1. Allgemeine Bewertung

Dieser Bereich enthält Anforderungen hinsichtlich der Dokumentation des Modells, der Nachvollziehbarkeit und Realisierbarkeit. Notwendige Kriterien sind u.a. Veröffentlichungen in Fachzeitschriften, Programmdokumentationen und Prüfbarkeit von Modell und Programm durch Dritte.

2.2. Wissenschaftliche Bewertung

Der Bereich der wissenschaftlichen Bewertung soll sicherstellen, dass das Modell von seinen physikalischen Grundlagen her für bestimmte Anwendungsbereiche geeignet ist. Die Anforderungen unterscheiden sich nach notwendigen Kriterien, die grundsätzlich vom Modell zu erfüllen sind, und optionalen Kriterien, die nur für spezielle Anwendungsbereiche erfüllt sein müssen.

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[3] Die in der aktuellen Programmversion implementierten Kriterien sind im Anhang A.2 aufgelistet. Da die Richtlinie 3783, Blatt 7 bei Fertigstellung dieses Programms noc nicht verabschiedet ist, können die entgültigen Kriterien von den hier implementierten abweichen. Die Kriterien entsprechen dem Stand der Richtlinie im November 2000.

Zu den notwendigen Kriterien zählen u.a. die Vollständigkeit des Gleichungssystems, zulässige Approximationen und Parameterisierungen. Dagegen stellt die im Modell ggf. enthaltene Wolkenmikrophysik ein optionales Kriterium dar, das nur dann erfüllt sein muss, wenn im Rahmen einer konkreten Modellanwendung Wolkenbildung berücksichtigt werden muß.

2.3. Validierung und Ergebniskontrolle

Unter der Validierung sind sieben Gruppen von Testfällen zusammengefasst, die vom Modell nachgerechnet werden müssen (Tabelle 1). Die Ergebnisse der hierfür insgesamt nötigen zwölf bzw. 13 Modellrechnungen werden je nach Testfall mit Modellergebnissen, analytischen Lösungen oder Naturdatensätzen verglichen, wobei die Bewertung anhand von Trefferquoten erfolgt. Für eine erfolgreiche Validierung muss in jedem einzelnen Testfall eine Trefferquote von mindestens 2/3 erreicht werden. Die erlaubten Abweichungen zwischen Modellergebnis und Referenzdaten sind abhängig vom Testfall und in der Richtlinie definiert.

Testfall	Art der Orographie / Bodennutzung	besonders untersuchte Eigenschaften	geänderter Parameter	Zahl Modell-rechnungen	Vergleichs-datensatz
a	homogenes Terrain	numerische Genauigkeit	Anström-richtung	5	Modellergebnis a1
b1	Bergrücken	Orographie-einfluss	-	1	analytische Lösung
b2	Bergrücken	Schichtungs- und Windge-schwindigkeits-einfluss	Wind-ge-schwindigkeit	2	analytische Lösung
c1	idealisierte Küste	Boden-temperatur	-	1	Plausibilitäts-prüfung
c2[4]	idealisierte Küste	Kondensation	-	1	Modellergebnis c1
d1	realer Hügel	Umströmungs-verhalten	-	1	Naturdatensatz
d2	Großraum Berlin	Tagesgang	-	1	Naturdatensatz

Tabelle 1: Testfälle der VDI 3783, Blatt 7

Die sieben Gruppen von Testfällen sollen möglichst isoliert einzelne Modelleigenschaften prüfen. Dazu zählen u.a. numerische Eigenschaften, orographische Effekte, Stabilitätseinflüsse und die realistische Berücksichtigung realer Orographien und Landnutzungen.

Weitere Anforderungen an das Modell sind in einer Liste von Kriterien zur Online- und Offline-Qualitätskontrolle der Modellergebnisse formuliert. Zu den Prüfpunkten zählen z.B. die Kontrolle auf numerisch bedingte Wellenbildung, Massenerhaltung oder Eigenschaften des verwendeten Modellgitters.

2.4. Abschließende Bewertung

Die Gesamtbewertung erfolgt anhand aller oben genannten Prüfkriterien. Der Modellanwender hat auf Basis der Ergebnisse aller Einzelprüfungen ein zusammenfassendes Evaluierungs-protokoll zu erstellen, in dem alle Prüfkriterien in Form einer Liste aufzuführen und mit „erfüllt“ oder „nicht erfüllt“ zu kennzeichnen sind. Das Modell gilt als im Sinne der Richtlinie evaluiert,

[4] Diese Testrechnung ist optional und muß nur durchgeführt werden, wenn das Modell auch hinsichtlich der Wolkenbildungsprozesse geprüft werden soll.

wenn es alle Prüfschritte erfolgreich durchlaufen hat. Wird ein Prüfpunkt nicht erfüllt, so ist das Modell nicht erfolgreich validiert und nur für die Anwendungsbereiche gültig, die durch die erfüllten Prüfkriterien abgedeckt werden.

3. Prüfung der Testfälle in EVA

Für jeden Testfall der Richtlinie hat der Anwender Modellergebnisdateien im EVA-Eingabeformat (Abschnitt 5.1.2 und Anhang A.1) bereitzustellen. Falls das Modell METRAS PC evaluiert werden soll, kann der Anwender auch direkt die Ausgabedateien des Modells bereitstellen. Diese werden von EVA in das EVA-Format konvertiert. Die Evaluierung erfolgt aber in jedem Fall anhand der Dateien im EVA-Format. Auf diese Weise ist sichergestellt, dass METRAS PC gegenüber anderen mesoskaligen Modellen gleichbehandelt wird und z.B. Trefferquoten nicht deshalb besser ausfallen, weil Interpolationen auf bestimmte Raum- oder Zeitpunkte überflüssig sind.

Die Auswertung der Testfallergebnisse zusammen mit den durch den Anwender angegebenen Modelleigenschaften (Abschnitt 5.1.1) wird im Laufzeitprotokoll (Abschnitt 5.2.1) in detaillierter Form und im Evaluierungszertifikat (Abschnitt 5.2.2) gemäß den Vorschriften der Richtlinie in zusammengefasster Form ausgegeben.

Soweit in den Abschnitten dieses Kapitels Bezug auf die Kriterien der VDI Richtlinie 3783 Blatt 7 genommen wird, können die in der aktuellen Programmversion implementierten Kriterien dem Anhang A.2 entnommen werden. An dieser Stelle sei nochmals darauf hingewiesen, dass sie dem Stand der Richtlinie vom November 2000 entsprechen.

3.1. Testfall a

Dieser Testfall umfasst fünf Dateien von Modellergebnissen, deren Inhalt und Reihenfolge der Bereitstellung in der Tabelle 2 angegeben sind.

Datei-Nr.	Inhalt
1	Referenzfall a1: Anströmrichtung 0°
2	Vergleichsfall a2: Anströmrichtung 45°
3	Vergleichsfall a3: Anströmrichtung 90°
4	Vergleichsfall a4: Anströmrichtung 180°
5	Vergleichsfall a5: Anströmrichtung 270°

Tabelle 2: Modellergebnisdateien Testfall a

Vom Programm EVA werden die folgenden Kriterien anhand der Richtlinienvorgaben geprüft bzw. berechnet:

Gitterstruktur

- Anzahl Modellgitterpunkte
- horizontale Gitterweiten Δx und Δy (Toleranz: +/- 2 m)
- minimale vertikale Gitterweite Δz (Toleranz: +/- 0.5 m)
- Oberrand des Modellgebiets mindestens 2500 m (Toleranz: 0 m)

Ausgabezeitpunkte

- Zeitintervall der Ausgabe (alle 3 Stunden bis 6 Stunden Modellintegrationszeit).

Plausibilitätskontrolle

- geographische Koordinaten, Höhe und Topographiehöhe an allen eingelesenen Gitterpunkten definiert?

- Gitterpunkte in Eingabedaten nicht doppelt vorhanden?

Vergleich Eingabedateien

- Reihenfolge und Koordinaten der Gitterpunkte mit Referenzfall a1 identisch?
- Modellzeiten mit Referenzfall identisch?

Trefferquoten

Ergibt die Prüfung aller vorstehenden Kriterien keinen Fehler, so werden die Trefferquoten[5] für alle in der Richtlinie definierten Vergleichsgrößen, deren Werte oberhalb der Nachweisgrenze liegen, unter Einbeziehung aller eingelesenen Gitterpunkte berechnet.

3.2. Testfall b1

Vom Programm werden die folgenden Kriterien anhand der Richtlinienvorgaben geprüft bzw. berechnet:

Gitterstruktur

- Anzahl Modellgitterpunkte
- horizontale Gitterweiten Δx und Δy (Toleranz: +/- 2 m)
- minimale vertikale Gitterweite Δz (Toleranz: +/- 0.5 m)
- Oberrand des Modellgebiets mindestens 2500 m (Toleranz: 0 m)
- Modelltopographie (Toleranz: +/- 0.1 m)

Ausgabezeitpunkte

- Zeitintervall der Ausgabe (alle 3 Stunden bis 9 Stunden Modellintegrationszeit).

Plausibilitätskontrolle

- geographische Koordinaten, Höhe und Topographiehöhe an allen eingelesenen Gitterpunkten definiert?
- Gitterpunkte in Eingabedaten nicht doppelt vorhanden?

Trefferquoten

Ergibt die Prüfung aller vorstehenden Kriterien keinen Fehler, so werden die Trefferquoten[6] für alle in der Richtlinie definierten Vergleichsgrößen, deren Werte oberhalb der Nachweisgrenze liegen berechnet. In die Berechnung einbezogen werden nur diejenigen Gitterpunkte, deren Koordinaten innerhalb des auszuwertenden Gebietsausschnitts liegen, also zwischen 1000 m und 6000 m über NN.

Im Testfall b1 werden als Referenzdaten an jedem eingelesenen Gitterpunkt die Werte der analytischen Long-Lösung (siehe [1]) unter Verwendung der Gitterpunktskoordinaten berechnet.

3.3. Testfall b2

Dieser Testfall umfasst zwei Dateien von Modellergebnissen, deren Inhalt und Reihenfolge der Bereitstellung in der Tabelle 3 angegeben sind.

---

[5] *Verwendete Prüfkriterien siehe Tabelle A.2.2.*

[6] *Verwendete Prüfkriterien siehe Tabelle A.2.3.*

Datei-Nr.	Inhalt
1	b2-1: geostrophischer Wind 10 m/s
2	b2-2: geostrophischer Wind 5 m/s

Tabelle 3: Modellergebnisdateien Testfall b2

Vom Programm werden die folgenden Kriterien anhand der Richtlinienvorgaben geprüft bzw. berechnet:

Gitterstruktur

- Anzahl Modellgitterpunkte
- horizontale Gitterweiten Δx und Δy (Toleranz: +/- 2 m)
- minimale vertikale Gitterweite Δz (Toleranz: +/- 0.5 m)
- Oberrand des Modellgebiets mindestens 2500 m (Toleranz: 0 m)
- Modelltopographie (Toleranz: +/- 0.1 m)

Ausgabezeitpunkte

- Zeitintervall der Ausgabe (alle 3 Stunden bis 9 Stunden Modellintegrationszeit).

Plausibilitätskontrolle

- geographische Koordinaten, Höhe und Topographiehöhe an allen eingelesenen Gitterpunkten definiert?
- Gitterpunkte in Eingabedaten nicht doppelt vorhanden?

Trefferquoten

Ergibt die Prüfung aller vorstehenden Kriterien keinen Fehler, so werden die Trefferquoten[7] für alle in der Richtlinie definierten Vergleichsgrößen, deren Werte oberhalb der Nachweisgrenze liegen berechnet. In die Berechnung einbezogen werden nur diejenigen Gitterpunkte, deren Koordinaten innerhalb des auszuwertenden Gebietsausschnitts liegen, also zwischen 1000 m und 6000 m über NN.

Im Testfall b2 werden als Referenzdaten an jedem eingelesenen Gitterpunkt die Werte der analytischen Long-Lösung unter Verwendung der Gitterpunktskoordinaten berechnet.

Wellenlängen

Zur Berechnung der Wellenlänge in den Modellergebnissen wird zunächst für die in der Mitte des Modellgebiets gelegene x-z-Schnittebene die Vertikalsäule bestimmt, in der die maximale Vertikalwindgeschwindigkeit auftritt. Innerhalb dieser Säule werden anschließend alle Gitterpunkte mit lokalem Minimum bzw. Maximum der Vertikalwindgeschwindigkeit bestimmt. Dabei erfolgt die Prüfung über die gesamte Höhe des Modellgebietes und beschränkt sich nicht nur auf den vertikalen Gebietsausschnitt, der zur Berechnung der übrigen Trefferquoten herangezogen wird. Die Wellenlänge ergibt sich aus der Mittelung aller Höhendifferenzen zwischen den Gitterpunkten benachbarter Minima und benachbarter Maxima.

Die Trefferquote für den Prüfpunkt „Wellenlänge“ ist 100 %, wenn die aus den Modellergebnissen berechnete Wellenlänge von der analytischen (vgl. [1]) um nicht mehr als 25 % abweicht. Dieser Prozentsatz entspricht der in der Richtlinie angegebenen absolut zulässigen Abweichung. Ist die Differenz größer, wird die Trefferquote auf 0 % gesetzt.

[7] *Verwendete Prüfkriterien siehe Tabelle A.2.4.*

3.4. Testfall c1

Vom Programm werden die folgenden Kriterien anhand der Richtlinienvorgaben geprüft bzw. berechnet:

Gitterstruktur

- Anzahl Modellgitterpunkte
- horizontale Gitterweiten Δx und Δy (Toleranz: +/- 2 m)
- minimale vertikale Gitterweite Δz (Toleranz: +/- 0.5 m)
- Oberrand des Modellgebiets mindestens 5000 m (Toleranz: 0 m)

Ausgabezeitpunkte

- Zeitintervall der Ausgabe (alle 4 Stunden bis 24 Stunden Modellintegrationszeit).

Plausibilitätskontrolle

- geographische Koordinaten, Höhe und Topographiehöhe an allen eingelesenen Gitterpunkten definiert?
- Gitterpunkte in Eingabedaten nicht doppelt vorhanden?

Trefferquoten

Ergibt die Prüfung aller vorstehenden Kriterien keinen Fehler, so wird mit der Berechnung der Trefferquote fortgesetzt. In diesem Testfall sieht die Richtlinie nur den Vergleich der Verlagerungsgeschwindigkeiten der Seewindfront zwischen den Zeitintervallen 12-16 Uhr und 16-20 Uhr vor. Wächst die Verlagerungsgeschwindigkeit zwischen den beiden Zeitintervallen (bei gleicher Verlagerungsrichtung) an, so liegt die Trefferquote bei 100 %, anderenfalls bei 0 %.

Die Position der Seewindfront zu den drei Ausgabezeiten 12, 16 und 20 Uhr wird in EVA anhand von vier Kriterien abgeschätzt:

1. Position der minimalen Divergenz (=maximale Konvergenz)
2. Position der maximalen positiven Vertikalwindgeschwindigkeit
3. Position des maximalen Gradienten der potentiellen Temperatur in y-Richtung
4. Position des maximalen Gradienten der relativen Feuchte in y-Richtung

Aus den so bestimmten (in der Regel nicht identischen) vier Positionen wird ein Mittelwert gebildet, wobei nur die Frontpositionen in die Mittelung eingehen, die um nicht mehr als 4 km von der aus der Divergenz bestimmten Frontposition abweichen. Schließlich wird die mittlere Frontgeschwindigkeit in den Zeitintervallen 12-16 Uhr und 16-20 Uhr aus den mittleren Frontpositionen berechnet.

3.5. Testfall c2

Vom Programm werden die folgenden Kriterien anhand der Richtlinienvorgaben geprüft bzw. berechnet:

Gitterstruktur

- Anzahl Modellgitterpunkte
- horizontale Gitterweiten Δx und Δy (Toleranz: +/- 2 m)
- minimale vertikale Gitterweite Δz (Toleranz: +/- 0.5 m)
- Oberrand des Modellgebiets mindestens 5000 m (Toleranz: 0 m)

Ausgabezeitpunkte

- Zeitintervall der Ausgabe (alle 4 Stunden bis 24 Stunden Modellintegrationszeit).

Plausibilitätskontrolle

- geographische Koordinaten, Höhe und Topographiehöhe an allen eingelesenen Gitterpunkten definiert?
- Gitterpunkte in Eingabedaten nicht doppelt vorhanden?

Trefferquoten

Ergibt die Prüfung aller vorstehenden Kriterien keinen Fehler, so wird mit der Berechnung der Trefferquote fortgesetzt. Wie schon im Testfall c1 ist das Prüfkriterium die Verlagerungsgeschwindigkeit der Seewindfront, die analog zu c1 im Programm berechnet wird. Zusätzlich müssen alle Verlagerungsgeschwindigkeiten und das Maximum der Vertikalwindgeschwindigkeit größer als in den jeweils korrespondierenden Zeiträumen des Testfalls c1 sein.

Wegen der Notwendigkeit des Vergleichs kann der Testfall c2 von EVA nur dann evaluiert werden, wenn gleichzeitig auch der Fall c1 evaluiert wird.

3.6. Testfälle d1 und d2

Der Testfall d1 umfasst zwei Dateien von Modellergebnissen, deren Inhalt und Reihenfolge der Bereitstellung in Tabelle 4 angegeben sind. Für den Testfall d2 ist nur eine Modellergebnisdatei vorgesehen.

Datei-Nr.	Inhalt
1	d1-1: neutrale Schichtung
2	d1-2: stabile Schichtung

Tabelle 4: Modellergebnisdateien Testfall d1

Vom Programm werden die folgenden Kriterien anhand der Richtlinienvorgaben geprüft bzw. berechnet:

Struktur und Inhalt der Modellergebnisdateien

Die Referenzdateien mit den Messdaten beider Testfälle werden mit EVA ausgeliefert (Dateien *d11.dat*, *d12.dat* und *d21.dat*; siehe Abschnitt 5.1.3). Die Modellergebnisse müssen vom Anwender hinsichtlich der Reihenfolge und Koordinaten der Messpunkte und Reihenfolge der Vergleichsgrößen identisch zu den Messdatendateien bereitgestellt werden. Ggf. sind hierzu Modellergebnisse auf die Messpunktkoordinaten und Messzeitpunkte zu interpolieren. Stimmen beide Dateien in ihrer Struktur nicht überein, so kann eine Evaluierung der Testfälle nicht durchgeführt werden.

Trefferquoten

Ergibt die Prüfung der Modellergebnisdateien hinsichtlich Struktur und Inhalt keinen Fehler, so werden die Trefferquoten[8] für alle in der Richtlinie definierten Vergleichsgrößen, deren Werte oberhalb der Nachweisgrenze liegen berechnet.

4. Statistische Analyse

Die VDI Richtlinie sieht neben der Bestimmung von Trefferquoten keine weitere Berechnung von statistischen Kenngrößen der Differenzen zwischen Modellergebnissen und Referenzdaten (Modellergebnis, analytische Lösungen oder Messdaten) vor. Gerade für den Fall, dass das Modell die vorgeschriebenen Trefferquoten nicht erreicht, ist es für den Anwender aber hilfreich, weitere Informationen zu den Abweichungen der Modellergebnisse zu erhalten. Für die Testfälle a, b und d werden von EVA daher einige statistische Größen, bezogen auf die Differenzen

[8] *Verwendete Prüfkriterien siehe Tabelle A.2.5, A.2.6.*

zwischen Modellergebnissen und Referenzdaten, berechnet. In den Testfällen c ist dies nicht möglich, weil hier kein direkter Datenvergleich, sondern nur eine Plausibilitätskontrolle durch die Richtlinie vorgeschrieben ist.

In die Berechnung von Trefferquoten gehen ebenso wie in die statistische Analyse nur solche Modellergebnisse *M* und Referenzdaten *R* ein, die oberhalb einer Nachweisgrenze R_0 liegen[9]. Für eine gegebene Vergleichsgröße (z.B. Windgeschwindigkeit oder potentielle Temperatur) liegen Daten oberhalb der Nachweisgrenze an *J* Gitter- bzw. Referenzpunkten vor. In die Berechnung von Trefferquoten und statistischer Analyse gehen dann alle Differenzen

$$D_j = \left| M_j - R_j \right| \quad j = 1, J$$

ein. Als Treffer zählen alle Datenpunkte mit $D_j < D_0$, wobei D_0 die erlaubte Abweichung der betrachteten Vergleichsgröße ist.

Die Richtlinie sieht als Ergebnis des Evaluierungsprozesses für einen Testfall nur die Aussage „Trefferquote >= 2/3“ oder „Trefferquote < 2/3“ vor. EVA gibt im Laufzeitprotokoll (Abschnitt 5.2.1) zusätzlich aus, welchen Prozentwert die Trefferquote für jede Vergleichsgröße erreicht. Darüber hinaus wird die mittlere Differenz

$$\overline{D} = \frac{1}{J} \sum_{j=1}^{J} D_j$$

und der mittlere quadratische Fehler aus den Differenzen

$$RMSE = \sqrt{\frac{1}{J} \sum_{j=1}^{J} \left(D_j\right)^2}$$

berechnet und im Laufzeitprotokoll ausgegeben. Falls das Modell die erforderliche Trefferquote nicht erreicht, können weitere Informationen hilfreich sein, wo die maximalen Differenzen auftreten und welche Form die Häufigkeitsverteilung der Differenzen hat. EVA gibt neben der minimalen Differenz $\min(D_j)$ auch die maximale Differenz $\max(D_j)$, deren Position in geographischen Koordinaten und Höhe, sowie den Zeitpunkt (Datum und Uhrzeit) aus. Schließlich wird die Häufigkeitsverteilung in den Differenzenklassen *n=0,N* bestimmt. Innerhalb jeder Klasse werden alle Differenzen D_j gezählt, die innerhalb der Klassengrenzen L_n liegen:

$$L_{n-1} \le D_j < L_n$$

Die Anzahl *N* und die Klassengrenze L_N können vom Anwender gewählt werden, die einzelnen Klassengrenzen werden vom Programm nach der Tabelle 5 festgelegt.

Klasse n	untere Grenze L_n	obere Grenze L_{n+1}
0	$-\infty$	*0*
1,...,N-1	$(n-1) * \frac{L_N}{N-1}$	$n * \frac{L_N}{N-1}$
N	L_N	$+\infty$

Tabelle 5: Klassengrenzen zur Bestimmung der Häufigkeitsverteilung von Differenzen

[9] *Die Nachweisgrenze ist nur für die Windrichtung ungleich Null (siehe Anhang A.2).*

Für L_N ist standardmäßig die erlaubte Abweichung D_0 vorzugeben. In diesem Fall werden alle „Treffer" in den Klassen *1* bis *N-1* gezählt. Eine feinere Analyse der „Nicht-Treffer" ist möglich, indem der Anwender einen Wert $L_N > D_0$ wählt.

Negative Differenzen D_j sind per Definition nicht möglich. Die Klasse 0 enthält daher all die Datenpunkte, die nicht definiert sind bzw. unterhalb der Nachweisgrenze liegen.

5. Dateien

5.1. EVA-Eingabedateien

5.1.1. Steuerdatei

Die Steuerung von EVA erfolgt über die Datei *eva.inp*[10], die im Laufverzeichnis von EVA vorliegen muss. Die Datei wird formatfrei eingelesen. Als Regeln für die Steuerdatei gelten:

- Innerhalb jeder Zeile werden alle Zeichen, die einem Ausrufezeichen („!") folgen, als Kommentar ignoriert.
- Eingaben sind durch `SCHLÜSSELWORT = SCHLÜSSELWERT` definiert
- Der Schlüsselwert beginnt mit dem ersten nicht leeren Zeichen nach Schlüsselwort und Gleichheitszeichen („=") und endet mit dem letzten Zeichen vor einem Leerzeichen („ „) oder Kommentarzeichen („!").
- Jede Zeile kann nur ein Schlüsselwort plus Schlüsselwert enthalten.
- Die Reihenfolge der Eingabedaten innerhalb der Steuerdatei ist beliebig.
- Schlüsselwörter und Schlüsselwerte können fehlen, soweit sie für die Evaluierungsrechnung ohne Bedeutung sind.

Interpretationsbeispiele für Schlüsselwerte sind in dem unten stehenden Dateibeispiel enthalten.

Beispiel für ein *eva.inp*:

```
!===============================================================================
!                EVA - Input Control File (eva.inp)
!===============================================================================
! Note: Lines starting with "!" are interpreted as comment lines.
!       Data lines must consist of KEY_WORD = KEY_VALUE.
!       KEY_VALUEs are read from the first non-blank character following "="
!       and end with the last character before the next blank or "!",
!       for example:
!       model_name      =  Model 1        (Result: "Model")
!       model_name      =  model !1       (Result: "model")
!       model_relperson = Jack the Ripper (Result: "Jack")
!       model_relperson = Jack_the_Ripper (Result: "Jack_the_Ripper")
!       model_version   = 2 .0            (Result: "2")
!       model_version   = 2.0             (Result: "2.0")
!       The sequence of data lines and comment lines is free.
!-------------------------------------------------------------------------------
!Part 0: Information on the Mesoscale Model
!-------------------------------------------------------------------------------
 proj_title      = evltst_1           ! titel of evaluation project
 proj_person     = Erika_Mustermann   ! person responsible for evaluation
 model_name      = ZISCH              ! name of model to be evaluated
 model_version   = 2.0                ! model version
 model_reldate   = 2001/07/31         ! model release date
 model_relperson = Hans_Mustermann    ! person responsible for model release
 model_supperson = Hans_Mustermann    ! person supporting model version
 eval_cert = D:\tmp\EVA\Results       ! Path to write evaluation certificate
 eval_rep  = D:\tmp\EVA\Reports       ! Path to write evaluation report
!-------------------------------------------------------------------------------
```

[10] *Die Datei wird nicht für die **METRAS⁺**-Version von EVA benötigt. In **METRAS⁺** werden die Steuerdaten über einen Eingabedialog bereitgestellt.*

```
!Part 1: General Assessment
!---------------------------------------------------------------------------
!
 doc_com         = yes                ! model comprehensible (yes/no)
 doc_short       = yes                ! short documentation (yes/no)
 doc_long        = yes                ! long documentation (yes/no)
 doc_man         = yes                ! user manual (yes/no)
 doc_tref        = no                 ! technical reference (yes/no)
!
!---------------------------------------------------------------------------
!Part 2: Scientific Assessment
!---------------------------------------------------------------------------
!
 prop_uvwprog    = yes                ! u,v,w wind prognostiv (yes/no)
 prop_tprog      = yes                ! T prognostic (yes/no)
 prop_qprog      = yes                ! q prognostic (yes/no)
 prop_conti      = yes                ! continuity equ./anelast.approx. (yes/no)
 prop_bouy       = yes                ! bouyancy forces (yes/no)
 prop_turpar     = yes                ! turbulence f(stability) (yes/no)
 prop_coriolis   = yes                ! Coriolis force (yes/no)
 prop_flxloc     = yes                ! flux steady f(location) (yes/no)
 prop_flxstab    = yes                ! flux steady f(stability) (yes/no)
 prop_flxmo      = yes                ! direct surf.flux or MO-theory
 prop_fritens    = yes                ! symmetric friction tensor (yes/no)
 prop_exphgt     = yes                ! explicit terrain height (yes/no)
 prop_rough      = yes                ! veget./build. as roughness (yes/no)
 prop_3dnoequi   = yes                ! 3d non-uniform grid (yes/no)
 prop_etacoor    = yes                ! surf. follow. coord. (yes/no)
 prop_cloud      = yes                ! cloud physics (yes/no)
 prop_ice        = yes                ! ice phase (yes/no)
 prop_subconv    = yes                ! subscale convection (yes/no)
 prop_surtemp    = yes                ! sur.flux w. force restore (yes/no)
 prop_surrad     = yes                ! sur.flux w. radiation (yes/no)
 prop_surincl    = yes                ! sur.flux w. inclin. (yes/no)
 prop_surshad    = yes                ! sur.flux w. shading (yes/no)
 prop_surhumid   = yes                ! sur.humidity prognostic(yes/no)
!
!---------------------------------------------------------------------------
!Part 3: Validation
!---------------------------------------------------------------------------
! Control of results (VDI guideline chapter 3.2)
!
 ctrl_grid       = yes                ! contr. of grid structure (yes/no)
 ctrl_2dt        = yes                ! contr. of 2*DT waves (yes/no)
 ctrl_sdev       = yes                ! contr. of std.deviation (yes/no)
 ctrl_aravg      = yes                ! contr. of area average (yes/no)
 ctrl_mass       = yes                ! contr. of mass (yes/no)
 ctrl_range      = yes                ! contr of val. range of values (yes/no)
 ctrl_2dxy       = yes                ! contr. of 2*DX/DY waves (yes/no)
 ctrl_indep      = yes                ! contr. of ind. from grid (yes/no)
 ctrl_plaus      = yes                ! contr. of results (yes/no)
!---------------------------------------------------------------------------
!Part 3a: Control of test case "a"
!---------------------------------------------------------------------------
a_run = 2                             ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
a_file1 = D:\tmp\EVA\Results\a1.efm   ! 1. model result file (or conv.METRAS result)
a_file2 = D:\tmp\EVA\Results\a2.efm   ! 2. model result file (or conv.METRAS result)
a_file3 = D:\tmp\EVA\Results\a3.efm   ! 3. model result file (or conv.METRAS result)
a_file4 = D:\tmp\EVA\Results\a4.efm   ! 4. model result file (or conv.METRAS result)
a_file5 = D:\tmp\EVA\Results\a5.efm   ! 5. model result file (or conv.METRAS result)
a_nclass_dd = 10                      ! dd: number of histogram classes
a_lowbnd_dd = 0.1                     ! dd: lower boundary of a_nclass_dd
a_nclass_ff = 10                      ! vv: number of histogram classes
a_lowbnd_ff = 0.005                   ! vv: lower boundary of a_nclass_ff
a_nclass_tp = 10                      ! tp: number of histogram classes
a_lowbnd_tp = 1.e-6                   ! tp: lower boundary of a_nclass_tp
! key_values if a_run = 2:
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm ! 1. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm ! 2. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm ! 3. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm ! 4. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm ! 5. METRAS result file
a_METturb   = 1                       ! 1=Luepkes/Schluenzen, 2=TKE
a_METcloud  = 0                       ! run without(=0)/with(=1) cloud physics
a_METtrace  = 0                       ! run without(=0)/with(>=1) no. of tracer
a_METntimes = 2                       ! number of output times (see a_METtimes)
```

```
a_METtimes  = 3.00                    ! 1. output time
a_METtimes  = 6.00                    ! 2. output time
!-------------------------------------------------------------------------------
!Part 3b1: Control of test case "b1"
!-------------------------------------------------------------------------------
b1_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
b1_file = D:\tmp\EVA\Results\b1.efm   ! model result file (or conv.METRAS result)
b1_nclass_dd = 10                     ! dd: number of histogram classes
b1_lowbnd_dd = 1.                     ! dd: lower boundary of b1_nclass_dd
b1_nclass_ff = 10                     ! vv: number of histogram classes
b1_lowbnd_ff = 0.05                   ! vv: lower boundary of b1_nclass_ff
b1_nclass_tp = 10                     ! tp: number of histogram classes
b1_lowbnd_tp = 1.e-6                  ! tp: lower boundary of b1_nclass_tp
! key_values if b1_run = 2:
b1_METfile = d:\tmp\METRAS\Results\AOutMVDI-b1_00000000-00090000.mfm ! METRAS result file
b1_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
b1_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
b1_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
b1_METntimes = 3                      ! number of output times (see b1_METtimes)
b1_METtimes  = 3.00                   ! 1. output time
b1_METtimes  = 6.00                   ! 2. output time
b1_METtimes  = 9.00                   ! 3. output time
!-------------------------------------------------------------------------------
!Part 3b2: Control of test case "b2"
!-------------------------------------------------------------------------------
b2_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
b2_file1 = D:\tmp\EVA\Results\b21.efm ! 1. model result file (or conv.METRAS result)
b2_file1 = D:\tmp\EVA\Results\b22.efm ! 2. model result file (or conv.METRAS result)
b2_nclass_dd = 10                     ! dd: number of histogram classes
b2_lowbnd_dd = 1.                     ! dd: lower boundary of b2_nclass_dd
b2_nclass_ff = 10                     ! vv: number of histogram classes
b2_lowbnd_ff = 0.05                   ! vv: lower boundary of b2_nclass_ff
b2_nclass_tp = 10                     ! tp: number of histogram classes
b2_lowbnd_tp = 0.01                   ! tp: lower boundary of b2_nclass_tp
! key_values if b2_run = 2:
b2_METfile1 = d:\tmp\METRAS\results\AOutMVDI-b21_00000000-00090000.mfm ! 1. METRAS result file
b2_METfile2 = d:\tmp\METRAS\results\AOutMVDI-b21_00000000-00090000.mfm ! 2. METRAS result file
b2_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
b2_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
b2_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
b2_METntimes = 3                      ! number of output times (see b2_METtimes)
b2_METtimes  = 3.00                   ! 1. output time
b2_METtimes  = 6.00                   ! 2. output time
b2_METtimes  = 9.00                   ! 3. output time
!-------------------------------------------------------------------------------
!Part 3c1: Control of test case "c1"
!-------------------------------------------------------------------------------
c1_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
c1_file = D:\tmp\EVA\Results\c1.efm   ! model result file (or conv.METRAS result)
! key_values if c1_run = 2:
c1_METfile = d:\tmp\METRAS\Results\AOutMVDI-c1_00000000-01000000.mfm ! METRAS result file
c1_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
c1_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
c1_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
c1_METntimes = 3                      ! number of output times (see c1_METtimes)
c1_METtimes  = 12.00                  ! 1. output time
c1_METtimes  = 16.00                  ! 2. output time
c1_METtimes  = 20.00                  ! 3. output time
!-------------------------------------------------------------------------------
!Part 3c2: Control of test case "c2"
!-------------------------------------------------------------------------------
c2_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
c2_file = D:\tmp\EVA\Results\c2.efm   ! model result file (or conv.METRAS result)
! key_values if c2_run = 2:
c2_METfile = d:\tmp\METRAS\Results\AOutMVDI-c2_00000000-01000000.mfm ! METRAS result file
c2_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
c2_METcloud  = 1                      ! run without(=0)/with(=1) cloud physics
c2_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
c2_METntimes = 3                      ! number of output times (see c2_METtimes)
c2_METtimes  = 12.00                  ! 1. output time
```

```
c2_METtimes  = 16.00                 ! 2. output time
c2_METtimes  = 20.00                 ! 3. output time
!-------------------------------------------------------------------------------
!Part 3d1: Control of test case "d1"
!-------------------------------------------------------------------------------
d1_run = 2                           ! 0=no evaluation
                                     ! 1=evaluation
                                     ! 2=convert METRAS results and evaluate
d1_file1 = D:\tmp\EVA\Results\d11.efm ! 1. model result file (or conv.METRAS result)
d1_file2 = D:\tmp\EVA\Results\d12.efm ! 2. model result file (or conv.METRAS result)
d1_nclass_dd = 10                    ! dd: number of histogram classes
d1_lowbnd_dd = 40.                   ! dd: lower boundary of d1_nclass_dd
d1_nclass_ff = 10                    ! vv: number of histogram classes
d1_lowbnd_ff = 1.5                   ! vv: lower boundary of d1_nclass_ff
d1_nclass_tt = 10                    ! tt: number of histogram classes
d1_lowbnd_tt = 2.                    ! tt: lower boundary of d1_nclass_tt
d1_nclass_rh = 10                    ! rh: number of histogram classes
d1_lowbnd_rh = 10.                   ! rh: lower boundary of d1_nclass_rh
d1_nclass_pp = 10                    ! pp: number of histogram classes
d1_lowbnd_pp = 1.7                   ! pp: lower boundary of d1_nclass_pp
! key_values if d1_run = 2:
d1_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-d11_00140000-00170000.mfm ! 1. METRAS result file
d1_METfile2 = d:\tmp\METRAS\Results\AOutMVDI-d12_00140000-00170000.mfm ! 2. METRAS result file
d1_METturb   = 1                     ! 1=Luepkes/Schluenzen, 2=TKE
d1_METcloud  = 0                     ! run without(=0)/with(=1) cloud physics
d1_METtrace  = 0                     ! run without(=0)/with(>=1) no. of tracer
d1_METntimes = 3                     ! number of output times (see d1_METtimes)
d1_METtimes  = 15.00                 ! 1. output time
d1_METtimes  = 16.00                 ! 2. output time
d1_METtimes  = 17.00                 ! 3. output time
!-------------------------------------------------------------------------------
!Part 3d2: Control of test case "d2"
!-------------------------------------------------------------------------------
d2_run = 2                           ! 0=no evaluation
                                     ! 1=evaluation
                                     ! 2=convert METRAS results and evaluate
d2_file = D:\tmp\EVA\Results\d2.efm  ! model result file (or conv.METRAS result)
d2_nclass_dd = 10                    ! dd: number of histogram classes
d2_lowbnd_dd = 40.                   ! dd: lower boundary of d2_nclass_dd
d2_nclass_ff = 10                    ! ff: number of histogram classes
d2_lowbnd_ff = 1.5                   ! ff: lower boundary of d2_nclass_ff
d2_nclass_tt = 10                    ! tt: number of histogram classes
d2_lowbnd_tt = 2.                    ! tt: lower boundary of d2_nclass_tt
d2_nclass_rh = 10                    ! rh: number of histogram classes
d2_lowbnd_rh = 10.                   ! rh: lower boundary of d2_nclass_rh
d2_nclass_pp = 10                    ! pp: number of histogram classes
d2_lowbnd_pp = 1.7                   ! pp: lower boundary of d2_nclass_pp
! key_values if d2_run = 2:
d2_METfile = d:\tmp\METRAS\Results\AOutMVDI-d11_00140000-00170000.mfm ! METRAS result file
d2_METturb   = 1                     ! 1=Luepkes/Schluenzen, 2=TKE
d2_METcloud  = 0                     ! run without(=0)/with(=1) cloud physics
d2_METtrace  = 0                     ! run without(=0)/with(>=1) no. of tracer
d2_METntimes = 3                     ! number of output times (see d2_METtimes)
d2_METtimes  = 15.00                 ! 1. output time
d2_METtimes  = 16.00                 ! 2. output time
d2_METtimes  = 17.00                 ! 3. output time
!-------------------------------------------------------------------------------
```

Erläuterung der Schlüsselwörter:

Schlüsselwort	*Erläuterungen*
	Allgemeine Informationen zum Evaluierungsprojekt:
proj_title	Kennung für das Projekt
proj_person	Verantwortliche Person für das Projekt
model_name	Name des zu evaluierenden Modells
model_version	Versionsnummer des zu evaluierenden Modells
model_reldate	Freigabedatum des Modells
model_relperson	Name der für die Modellentwicklung verantwortlichen Person
model_supperson	Name der für den Modellsupport verantwortlichen Person
eval_cert	Ausgabepfad für das Evaluierungszertifikat
eval_rep	Ausgabepfad für das Laufzeitprotokoll
	Modelldokumentationen gemäß Kapitel 1 der VDI Richtlinie: Als Schlüsselwerte sind *yes* (=liegt vor bzw. ist erfüllt) oder *no* (=liegt nicht

	vor bzw. nicht erfüllt) möglich.
doc_com	Modell für Dritte nachvollziehbar
doc_short	Kurzfassung Modelldokumentation
doc_long	Langfassung Modelldokumentation
doc_man	Benutzerhandbuch
doc_tref	Technische Modellreferenz
	Notwendige Modelleigenschaften gemäß Kapitel 2 der VDI Richtlinie: Als Schlüsselwerte sind *yes* (=liegt vor bzw. ist erfüllt) oder *no* (=liegt nicht vor bzw. nicht erfüllt) möglich.
prop_uvwprog	Windkomponenten prognostisch
prop_tprog	Temperatur prognostisch
prop_qprog	spezifische Feuchte prognostisch
prop_conti	Kontinuitätsgleichung oder anelastische Approximation
prop_bouy	Auftriebskräfte
prop_turpar	Turbulenzparametrisierung stabilitätsabhängig
prop_coriolis	Corioliskraft
prop_flxloc	Flüsse stetig als Funktion des Ortes
prop_flxstab	Flüsse stetig als Funktion der Stabilität
prop_flxmo	direkte Berechnung oberflächennaher Flüsse / Monin-Obukhov-Theorie
prop_fritens	symmetrischer Spannungstensor
prop_exphgt	Geländehöhen explizit
prop_rough	Bewuchs / Bebauung als Rauhigkeit
prop_3dnoequi	dreidimensional nichtäquidistantes Gitter
prop_etacoor	bodenfolgendes Koordinatensystem
prop_cloud	Wolkenmikrophysik
prop_ice	Eisphase
prop_subconv	subskalige Konvektion
prop_surtemp	Bodenflüsse mindestens „force-restore“
prop_surrad	Bodenenergiebilanz einschl. Strahlung
prop_surincl	Bodenenergiebilanz einschl. Hangneigung
prop_surshad	Bodenenergiebilanz einschl. Abschattung
prop_surhumid	Bodenfeuchtebilanz
	Kontrolle der Modellergebnisse gemäß Kapitel 3.2 der VDI Richtlinie: Als Schlüsselwerte sind *yes* (=liegt vor bzw. ist erfüllt) oder *no* (=liegt nicht vor bzw. nicht erfüllt) möglich.
ctrl_grid	Gitterstruktur
ctrl_2dt	2*DT Wellen
ctrl_sdev	Standardabweichungen
ctrl_aravg	Flächenmittelwerte
ctrl_mass	Massenerhaltung
ctrl_range	Gültigkeitsbereiche (plausible Werte)
ctrl_2dxy	2*DX, 2*DY Wellen
ctrl_indep	Ergebnisse gitterunabhängig
ctrl_plaus	Ergebniskontrolle
	Testfälle a bis d gemäß Kapitel 3.1.1 der VDI Richtlinie: Die Platzhalter in den Schlüsselworten sind abhängig vom Testfall wie folgt zu ersetzen: *X*: Kürzel des Testfalls (*a, b1, b2, c1, c2, d1* oder *d2*) *N*: Anzahl von Dateien (a:*5*, b2:*2*, d1:*2*, in den anderen Fällen entfällt *N*) *KK*: Kürzel für Vergleichsgröße. Die für jeden Testfall vorgesehenen Vergleichsgrößen können dem Anhang A.2 entnommen werden. Allgemein ist für *KK* in EVA vorgesehen: *DD*: Windrichtung *FF*: Windgeschwindigkeit

	UU: u-Windkomponente *VV*: v-Windkomponente *WW*: w-Windkomponente *DV*: Divergenz *TP*: potentielle Temperatur *TT*: Realtemperatur *RH*: relative Feuchte *PP*: Druck
*X*_run	= 0: keine Evaluierung dieses Testfalls = 1: Evaluierung = 2: Evaluierung mit vorheriger Konvertierung von METRAS PC Ergebnis-dateien
	Die folgenden Schlüsselwerte müssen nur bei *X*_run > 0 angegeben werden:
*X*_file*N*	Pfad und Name der Modellergebnisdateien. Bei Konvertierung von METRAS PC Dateien werden die konvertierten Daten in diese Dateien geschrieben.
*X*_nclass_*KK*	Anzahl der Histogrammklassen für statistische Analyse (nicht für Testfälle c1, c2)
*X*_lowbnd_*KK*	untere Grenze der letzten Klasse (nicht für Testfälle c1, c2)
	Die folgenden Schlüsselwerte müssen nur angegeben werden, wenn METRAS PC Dateien konvertiert werden sollen (*X*_run=2):
*X*_METfile*N*	Pfad und Name der METRAS PC Ergebnisdateien
*X*_METturb	in den Simulationen verwendete Turbulenzparametrisierung = 1: nach Lüpkes/Schlünzen = 2: TKE
*X*_METcloud	Simulation erfolgte ohne (=0) oder mit (=1) Wolkenphysik
*X*_METtrace	Simulation erfolgte ohne (=0) oder mit (=1) Stofftransport
*X*_METntimes	Anzahl der auszuwertenden Ausgabezeiten (muss identisch mit den Vor-gaben der Richtlinie sein, unabhängig davon, wie viele Ausgabezeiten in den Dateien enthalten sind)
*X*_METtimes	*X*_METtimes Ausgabezeiten, die auszuwerten sind. Für jede Ausgabezeit ist eine eigene Zeile erforderlich.

5.1.2. Modellergebnisdateien

Wie viele und welche Modellergebnisdateien einer EVA-Rechnung bereitgestellt werden müssen ist abhängig von den Schlüsselwerten *X*_run in der Steuerdatei[11].

Ergebnisdateien anderer Modelle als METRAS PC müssen im EVA-Dateiformat, das im Anhang A.1 erläutert wird, vorliegen. Speziell für die Testfälle d1 und d2 gilt, dass nicht nur das Dateiformat eingehalten werden muss, sondern dass die Reihenfolge der Messpunkte und die Zeitangaben entsprechend der Reihenfolge in den Dateien mit den Referenzdaten (Abschnitt 5.1.3) eingehalten werden muss (vgl. Abschnitt 3.6).

Ergebnisdateien[12] von METRAS PC [2] müssen nicht für EVA aufbereitet werden. Sie werden programmintern in das erforderliche Format konvertiert und ausgegeben. Sind diese Dateien bereits bei einer früheren EVA-Rechnung konvertiert worden, so ist eine erneute Konvertierung nicht notwendig.

---

[11] *in der* ***METRAS+****-Version von EVA abhängig von den korrespondierenden Werten im Eingabedialog*

[12] *In der* ***METRAS+****-Version von METRAS PC werden diese Dateien standardmäßig mit der Endung *.mfm gespeichert.*

5.1.3. Messdaten der Testfälle d1 und d2

Die VDI Richtlinie 3783 Blatt 7 legt für die Testfälle d1 und d2 Referenzdatensätze (Messdaten) fest. Diese Datensätze werden mit EVA ausgeliefert und liegen nach erfolgreicher Installation im Installationsverzeichnis unter den Dateinamen

- *d11.dat* 1. Referenzdatensatz für Testfall d1 (neutrale Schichtung)
- *d12.dat* 2. Referenzdatensatz für Testfall d1 (stabile Schichtung)
- *d21.dat* Referenzdatensatz für Testfall d2

vor. Es handelt sich um lesbare ASCII-Dateien, die dem EVA-Format des Anhangs A.1 entsprechen. Mit jedem Programmstart von EVA werden diese Dateien auf Authentizität überprüft. Falls der Anwender beim Ansehen der Dateiinhalte versehentlich Änderungen vorgenommen und diese gespeichert hat, muss EVA neu installiert werden.

5.2. EVA-Ausgabedateien

5.2.1. Laufzeitprotokoll

Jede Rechnung mit EVA erzeugt im Laufverzeichnis ein Laufzeitprotokoll mit dem Namen eva*.erp*[13], in dem die Steuerdaten aufgelistet und alle wesentlichen Arbeitsschritte des Programms dokumentiert werden. Zusätzlich enthält das Laufzeitprotokoll die Ergebnisse der statistischen Analysen für die Testfälle a, b und d (Abschnitt 4).

Beispiel für ein Laufzeitprotokoll:

```
****** EVA started at 2001-07-30 21:27:58
       --------------------------------------
       | Meaning of following messages:       |
       | I#nnn:         info  message no. nnn |
       | W#nnn: warning error message no. nnn |
       | F#nnn: fatal   error message no. nnn |
       --------------------------------------
I#100: ===================================================================
       !     ***** Control data of this evaluation project: *****          !
       !                                                                   !
       ! -----------------------------------------------------------------
       ! 1. General Information
       ! -----------------------------------------------------------------
       ! Evaluation project             = evltst_2
       ! Person responsible             = Erika_Mustermann
       ! Model name                     = METRAS_PC
       ! Model version                  = 2.00Beta
       ! Model release date             = 2001/07/31
       ! Person responsible for release = Hans_Mustermann
       ! Person responsible for support = Hans_Mustermann
       ! File with Evaluation Certificate:
       !  --> d:\tmp\EVA\Results\evltst_2.ece
       ! File with Evaluation Report:
       !  --> d:\tmp\EVA\Reports\evltst_2.erp
       ! -----------------------------------------------------------------
       ! 2.a Properties of model to be evaluated: Documentation
       ! -----------------------------------------------------------------
       ! Model comprehensible ........................... = YES
       ! Documentation, short version ................... = YES
       ! Documentation, long version .................... = YES
       ! User manual .................................... = YES
       ! Technical reference ............................ = YES
       ! -----------------------------------------------------------------
       ! 2.b Properties of model to be evaluated: Implementation
       ! -----------------------------------------------------------------
       ! Three wind components prognostic ............... = YES
       ! Temperature prognostic ......................... = YES
       ! Specific humidity prognostic ................... = YES
       ! Continuity equation or anelstic approximation ... = YES
```

[13] *In der **METRAS**$^{+}$-Version wird das Protokoll unter einem anderen Namen abgelegt und enthält teilweise andere Einträge.*

```
! Buoyancy forces (eg. Boussinesq approximation) .. = YES
! Turbulence parameterization function of stability = YES
! Coriolis force ................................. = YES
! Fluxes steady (function of location) ........... = YES
! Fluxes steady (function of stability) .......... = YES
! Direct calculation of surface fluxes or MO theory = YES
! Symmetric friction tensor ...................... = YES
! Explicit elevation heights ..................... = YES
! Canopy/buildings as roughness lengths .......... = YES
! 3d non-equidistant grid ........................ = YES
! Surface following coordinates .................. = YES
! Cloud physic / short & longwave radiation ....... = YES
! Ice phase prognostic ........................... = YES
! Parameterization of subgrid scale convection ......... = YES
! Surface temperature at least with force restore = YES
! Surface fluxes with short & longwave radiation .. = YES
! Surface fluxes with surface inclination ......... = YES
! Surface fluxes with shading ................... = YES
! Surface humidity balance ....................... = YES
! ------------------------------------------------------------------
! 2.c Properties of model to be evaluated: Result Control
! ------------------------------------------------------------------
! Grid structure ................................. = YES
! On-line control: 2*DT waves .................... = YES
! On-line control: standard deviations ........... = YES
! On-line control: area averages ................. = YES
! On-line control: constant mass ................. = YES
! On-line control: valid ranges .................. = YES
! Off-line control: 2*DX & 2*DY waves ............ = YES
! Off-line control: result independent from grid .. = YES
! Off-line control: comparison / plausible results  = YES
! ------------------------------------------------------------------
! 3. Control of test case "a"
! ------------------------------------------------------------------
! Test case "a" selected for evaluation
! Conversion of METRAS result files to EVA format:
!  --> D:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm
!  --> D:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm
!  --> D:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm
!  --> D:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm
!  --> D:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm
! Parameters of METRAS result file(s):
!  turbulence parameterization = Luepkes/Schluenzen
!  run with cloud physics      = NO
!  number of tracer            =  0
!  number of conversion times  =  2
!  conversion time no.  1      =   3.000000
!  conversion time no.  2      =   6.000000
! Model result file(s) in EVA format:
! (Result of METRAS file conversion)
!  --> D:\tmp\EVA\Results\VDI-a11
!  --> D:\tmp\EVA\Results\VDI-a12
!  --> D:\tmp\EVA\Results\VDI-a13
!  --> D:\tmp\EVA\Results\VDI-a14
!  --> D:\tmp\EVA\Results\VDI-a15
! Classes defined for statistical analysis:
! (Note: Whatever is listed here - statistical analysis is done
!        for those meteorological quantities only, which are part
!        of the evaluation process. However, statistical analysis
!        is NO part of the evaluation process but for user
!        information and error analysis!)
! Key - no.of classes - lower boundary of highest class
! DD    10                  0.100000000000
! FF    10                  0.005000000000
! TP    10                  0.000001000000
! ------------------------------------------------------------------
! 4. Control of test case "b1"
! ------------------------------------------------------------------
! Test case "b1" not selected for evaluation
! ------------------------------------------------------------------
! 5. Control of test case "b2"
! ------------------------------------------------------------------
! Test case "b2" not selected for evaluation
! ------------------------------------------------------------------
! 6. Control of test case "c1"
! ------------------------------------------------------------------
! Test case "c1" not selected for evaluation
! ------------------------------------------------------------------
```

```
       ! 7. Control of test case "c2"
       ! ------------------------------------------------------------------
       ! Test case "c2" not selected for evaluation
       ! ------------------------------------------------------------------
       ! 8. Control of test case "d1"
       ! ------------------------------------------------------------------
       ! Test case "d1" not selected for evaluation
       ! ------------------------------------------------------------------
       ! 9. Control of test case "d2"
       ! ------------------------------------------------------------------
       ! Test case "d2" not selected for evaluation
I#101: !                                                                  !
       !   ***** End of control data of this evaluation project *****     !
       ====================================================================
I#204: $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
       $                                 $
       $ Start processing test case "a " $
       $                                 $
       $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a11
I#111: File reading completed for file
       D:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a11
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a12
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a12
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a13
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a13
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a14
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a14
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a15
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a15
```

```
I#206: ===== METRAS data conversion completed
I#207: >>>>> Rearrange data for statistical evaluation.
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a11
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a12
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a13
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a14
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a15
I#107: Open output file:
       a.cdd
I#107: Open output file:
       a.cff
I#107: Open output file:
       a.ctp
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a11
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a11
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a12
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a12
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a13
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a13
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a14
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a14
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a15
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a15
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#231: >>>>> Start checking model grid
       Horizontal grid spacing in x-direction:
         Minimum Delta-x (m)     :  1999.485360236082
            (Number of occurences:  1 ;
            first occurence      :  ix,ix+1,iy = 10 11 15 )
         Maximum Delta-x (m)     :  1999.835902171675
            (Number of occurences:  1 ;
            first occurence      :  ix,ix+1,iy = 10 11 14 )
       Horizontal grid spacing in y-direction:
         Minimum Delta-y (m)     :  1999.803937169723
            (Number of occurences:  2 ;
            first occurence      :  ix,iy,iy+1 = 10 1 2 )
         Maximum Delta-y (m)     :  2000.237746986561
            (Number of occurences:  2 ;
            first occurence      :  ix,iy,iy+1 = 3 19 20 )
       Vertical grid spacing:
         Minimum Delta-z (m)     :  20.00000000000000
            (Number of occurences:  2000 ;
            first occurence      :  ix,iy,iz,iz+1 = 1 1 1 2 )
         Maximum Delta-z (m)     :  500.0000000000000
```

```
          (Number of occurences:  4400 ;
          first occurence      :  ix,iy,iz,iz+1 = 1 1 24 25 )
       I N F O:
       Maximum of vertical extent of model
       simulation domain as estimated by
       z(k_max)+0.5*[z(k_max)-z(k_max-1)]=  8674.000000000000  m
       satisfies value ( 2500.000000000000  m) required
       by the guideline.
       (Note: z(k) is height above ground.)
I#232: ===== Checking model grid completed successfully.
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a11
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a12
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a13
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a14
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a15
I#113: Writing to converted-data files completed.
I#130: Model data / ff-values: defined at all points for all times.
I#130: Model data / dd-values: defined at all points for all times.
I#130: Model data / tp-values: defined at all points for all times.
I#208: ===== Data conversion completed.
I#210: >>>>> Start statistical evaluation.

       ***************************************************
       ***** Start evaluating "Wind direction (°)"
       ***************************************************

       Allowed deviation:  0.1000000000000000
       Width of classes:  1.1111111111111111E-02

       Frequency Distribution of Differences
       - - - - - - - - - - - - - - - - - - -
       class           sum of
       index   counts   counts   relsum(%)    class boundaries [lower/upper)
       ---------------------------------------------------------------------
          00        0        0      0.00 -999.000000000000    0.000000000000 (undefined)
       ---------------------------------------------------------------------
          01    55200    55200     75.00    0.000000000000    0.011111111111 )
          02        0    55200      0.00    0.011111111111    0.022222222222 )
          03        0    55200      0.00    0.022222222222    0.033333333333 )
          04     8800    64000     11.96    0.033333333333    0.044444444444 )
          05     7600    71600     10.33    0.044444444444    0.055555555556 ) within
          06      400    72000      0.54    0.055555555556    0.066666666667 ) criterion
          07        0    72000      0.00    0.066666666667    0.077777777778 )
          08        0    72000      0.00    0.077777777778    0.088888888889 )
          09        0    72000      0.00    0.088888888889    0.100000000000 )
       ---------------------------------------------------------------------
          10     1600    73600      2.17    0.100000000000 9999.000000000000 (above criterion)
       ---------------------------------------------------------------------
       minimum difference      :    0.0000000000
       maximum difference      :    0.1259011225
         -> at lat,lon,z       :         49.99070          9.26505        683.00000
         -> value at lat,lon,z :  359.8672847926
         -> at date            :        99999999
         -> at output time     :           06:00
       mean difference         :    0.0127234826
       rmse                    :    0.0275433350

       ++ Hit rate for currently processed quantity : 97.82608695652173  %
          (number of hits : total number of defined cases = 72000 : 73600 )

       !! Overall hit rate after evaluating "DD": 97.826 %

       ***************************************************
       ***** Start evaluating "Wind speed (m/s)"
       ***************************************************

       Allowed deviation:  5.0000000000000000E-03
       Width of classes:  5.5555555555555556E-04

       Frequency Distribution of Differences
       - - - - - - - - - - - - - - - - - - -
       class           sum of
       index   counts   counts   relsum(%)    class boundaries [lower/upper)
```

```
      ---------------------------------------------------------------------
         00        0        0      0.00 -999.000000000000    0.000000000000 (undefined)
      ---------------------------------------------------------------------
         01    55200    55200     75.00    0.000000000000    0.000555555556 )
         02        0    55200      0.00    0.000555555556    0.001111111111 )
         03     1600    56800      2.17    0.001111111111    0.001666666667 )
         04     4400    61200      5.98    0.001666666667    0.002222222222 )
         05     3200    64400      4.35    0.002222222222    0.002777777778 ) within
         06     6000    70400      8.15    0.002777777778    0.003333333333 ) criterion
         07      800    71200      1.09    0.003333333333    0.003888888889 )
         08     1600    72800      2.17    0.003888888889    0.004444444444 )
         09        0    72800      0.00    0.004444444444    0.005000000000 )
      ---------------------------------------------------------------------
         10      800    73600      1.09    0.005000000000 9999.000000000000 (above criterion)
      ---------------------------------------------------------------------
      minimum difference      :    0.0000000000
      maximum difference      :    0.0073550356
        -> at lat,lon,z       :         50.00899          9.01396        819.50000
        -> value at lat,lon,z :    4.9961732872
        -> at date            :        99999999
        -> at output time     :           06:00
      mean difference         :    0.0007138812
      rmse                    :    0.0015360527

      ++ Hit rate for currently processed quantity : 98.91304347826087  %
         (number of hits : total number of defined cases = 72800 : 73600 )

      !! Overall hit rate after evaluating "FF": 97.826 %

      ***************************************************
      ***** Start evaluating "Potential temperature (K)"
      ***************************************************

      Allowed deviation:  1.000000000000000E-06
      Width of classes:  1.111111111111111E-07

      Frequency Distribution of Differences
      - - - - - - - - - - - - - - - - - - -
      class           sum of
      index   counts   counts   relsum(%)    class boundaries [lower/upper]
      ---------------------------------------------------------------------
         00        0        0      0.00 -999.000000000000    0.000000000000 (undefined)
      ---------------------------------------------------------------------
         01    73600    73600    100.00    0.000000000000    0.000000111111 )
         02        0    73600      0.00    0.000000111111    0.000000222222 )
         03        0    73600      0.00    0.000000222222    0.000000333333 )
         04        0    73600      0.00    0.000000333333    0.000000444444 )
         05        0    73600      0.00    0.000000444444    0.000000555556 ) within
         06        0    73600      0.00    0.000000555556    0.000000666667 ) criterion
         07        0    73600      0.00    0.000000666667    0.000000777778 )
         08        0    73600      0.00    0.000000777778    0.000000888889 )
         09        0    73600      0.00    0.000000888889    0.000001000000 )
      ---------------------------------------------------------------------
         10        0    73600      0.00    0.000001000000 9999.000000000000 (above criterion)
      ---------------------------------------------------------------------
      minimum difference      :    0.0000000000
      maximum difference      :    0.0000000000
        -> at lat,lon,z       :       -999.00000       -999.00000       -999.00000
        -> value at lat,lon,z : -999.0000000000
        -> at date            :            -999
        -> at output time     :            -999
      mean difference         :    0.0000000000
      rmse                    :    0.0000000000

      ++ Hit rate for currently processed quantity : 100.0000000000000  %
         (number of hits : total number of defined cases = 73600 : 73600 )

      !! Overall hit rate after evaluating "TP": 97.826 %

      $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
      $ Test case a (VDI-Guideline) - Overall hit rate :  97.826 % $
      $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

      ===== Statistical evaluation completed (a).
I#211: ===== Statistical evaluation completed.
I#216: 0 warning errors detected.
I#999: Execution completed. No fatal error detected.
****** EVA completed at 2001-07-30 21:30:50
```

Erläuterungen:

Meldungsnummer	Erläuterung
I#100 / I#101	Auflistung der Eingabedaten.
I#204	Abarbeitung eines Testfalls wird begonnen.
I#205	Konvertierung einer METRAS PC Ausgabedatei in das EVA-Format beginnt. Während der Konvertierung wird eine temporäre Datei *RMD.tmp* im Laufverzeichnis angelegt, deren Inhalt bei Problemen mit der Konvertierung Hinweise auf Fehlerursachen geben kann. Diese Datei wird mit jeder neuen Konvertierung überschrieben.
I#105	METRAS PC Ausgabedatei wird geöffnet.
I#107	Konvertierungsdatei wird geöffnet.
I#111	METRAS PC Ausgabedatei ist vollständig gelesen worden.
I#112	Konvertierungsdatei ist vollständig geschrieben worden.
I#206	Konvertierung der METRAS PC Ausgabedatei abgeschlossen.
I#207	Zur Berechnung der Trefferquoten werden temporäre Dateien angelegt, in denen Referenz- und Modelldaten neu sortiert werden
I#105	Modellergebnisdateien (EVA-Format) werden zum Lesen geöffnet.
I#107	Für jede Vergleichsgröße wird eine temporäre Datei angelegt.
I#230	Die Gitterkoordinaten in einer Modellergebnisdatei (EVA-Format) werden überprüft.
I#109	Einlesen zur Prüfung der Gitterkoordinaten beendet.
I#130	Geographische Koordinaten, Höhen und Topographiehöhe sind an allen Gitterpunkten definiert.
I#231	Die Gitterstruktur in allen Modellergebnisdateien wird auf Übereinstimmung mit den Anforderungen der Richtlinie überprüft: Meldung über die gefundenen minimalen und maximalen Gitterweiten und deren Lage im Gitter. Geringfügige Abweichungen gegenüber den im Modell verwendeten Werten können auf Rundungsfehlern und Modellausgabeformaten beruhen.
I#232	Prüfung der Gitterstruktur erfolgreich abgeschlossen.
I#109	Einlesen zur Prüfung der Gitterstruktur beendet.
I#113	Schreiben der temporären Dateien abgeschlossen.
I#130	Vergleichsgrößen an allen Punkten definiert.
I#208	Sortierung von Referenz- und Modelldaten in temporären Dateien abgeschlossen.
I#210	Ausgabe von Trefferquoten und Ergebnissen der statistischen Analyse für den aktuellen Testfall. Für jede Vergleichsgröße wird ausgegeben: - Nach Richtlinie erlaubte Abweichung der Vergleichsgröße von den Referenzdaten und (vom Anwender gewählte) Klassenbreite für das Histogramm der Differenzen. - Histogramm der absoluten Differenzen zwischen Modell- und Referenzdaten. Innerhalb jeder Klasse werden die Anzahl der Gitterpunkte, und deren prozentualer Anteil sowie die Klassengrenzen angegeben. Die Klasse 0 beinhaltet alle nicht definierten Datenpunkte, die höchste Klasse (im vorliegenden Fall) alle Punkte, die nicht innerhalb der erlaubten Abweichung liegen. - minimale und maximale absolute Differenz sowie deren Lage - mittlere absolute Differenz und RMSE - Trefferquote für diese Vergleichsgröße - Gesamttrefferquote nach Berechnung der aktuellen Vergleichsgröße. Die Gesamttrefferquote ist immer das Minimum aller bisher berechneten Trefferquoten.
I#211	Berechnung von Trefferquoten und statistische Analyse abgeschlossen.
I#216 / I#999	Es wurden keine Warnmeldungen oder fatale Fehler festgestellt.

5.2.2. Evaluierungszertifikat

Nach erfolgreicher Berechnung des Programms EVA wird ein Evaluierungszertifikat erstellt, dessen Name sich aus der Projektkennung (proj_title) und einer Endung „.ece“ zusammensetzt. Das Evaluierungszertifikat wird auch dann erstellt, wenn nicht alle Kriterien der Richtlinie erfüllt sind. Es kann in ausgedruckter und unterschriebener Form gegenüber Auftraggebern und Behörden als Nachweis dienen, dass das mesoskalige Modell gemäß der VDI Richtlinie 3783 Blatt 7 evaluiert worden ist.

Beispiel für ein Evaluierungszertifikat:

```
==============================================================================================
            Model Evaluation Certificate in Accordance with VDI Guideline 3783 Sheet7
==============================================================================================
This document certifies the evaluation of a prognostic mesoscale non-hydostatic wind field
model for dynamically and thermally driven wind fields. The certificate is in accordance with
VDI guideline 3783 Sheet7 (Nov.2000). Numbers in brackets [...] denote the corresponding
section of the guideline. Essential qualities are denoted "E", application dependent
qualities with "A".

----------------------------------------------------------------------------------------------
0. Information on the Mesoscale Model:
----------------------------------------------------------------------------------------------
   Name................................: ZISCH
   Version.............................: 2.00
   Release Date........................: 2001/07/31
   Responsible Person..................: Erika_Mustermann
   Responsible Person for this Evaluation: Hans_Mustermann
1. General Assessment:                                     [guideline]                  PASSED
----------------------------------------------------------------------------------------------
   E: Comprehensibility                                    [1.1]                        YES
   E: Documentation, short version                         [1.2.1]                      YES
   E: Documentation, long version                          [1.2.2]                      YES
   E: User Manual                                          [1.2.3]                      YES
   A: Technical Reference                                  [1.2.4]                      NO ***
----------------------------------------------------------------------------------------------
2. Scientific Assessment:                                  [guideline]                  PASSED
----------------------------------------------------------------------------------------------
   E: three wind components prognostic                     [2]                          NO ***
   E: temperature prognostic                               [2]                          YES
   E: specific humidity prognostic                         [2]                          YES
   E: continuity equation or anelastic approximation       [2]                          YES
   E: buoyancy forces (eg. Boussinesq approx.)             [2]                          YES
   E: turbulence parameterization function of stability    [2]                          YES
   E: Coriolis force considered                            [2]                          YES
   E: fluxes steady as function of location                [2]                          YES
   E: fluxes steady as function of stability               [2]                          YES
   E: direct calc. of surfaces fluxes or MO-theory         [2]                          YES
   E: symmetry of friction tensor                          [2]                          YES
   E: orography explicitly considered                      [2]                          YES
   E: vegetation and buildings as roughness lengths        [2]                          YES
   E: 3d non-uniform grid                                  [2]                          NO ***
   A: surface following coordinates                        [2]                          NO ***
   A: cloud physics / short and longwave radiation         [2]                          YES
   A: ice phase prognostic                                 [2]                          YES
   A: parameterization of sub-grid scale convection        [2]                          YES
   A: surface temperature prognostic                       [2]                          YES
   A: surface fluxes with short and lonwave radiation      [2]                          YES
   A: surface fluxes with surface inclination              [2]                          YES
   A: surface fluxes with shading by mountains             [2]                          YES
   A: surface humidity prognostic                          [2]                          NO ***
----------------------------------------------------------------------------------------------
3. Validation:                                             [guideline]                  PASSED
----------------------------------------------------------------------------------------------
   E: test case a -homogenous terrain                      [3.1.1]                      NO ***
   E: test case b1-mountain ridge/eff. of surface shape    [3.1.1]                      NO ***
   E: test case b2-mountain ridge/eff. of wind speed       [3.1.1]                      NO ***
   E: test case c1-idealized coast/eff. of surf. temp.     [3.1.1]                      NO ***
   E: test case c2-idealized coast/effect of clouds        [3.1.1]                      NO ***
   E: test case d1-field campaign Sophienhoehe             [3.1.1]                      NO ***
   E: test case d2-field campaign Berlin                   [3.1.1]                      NO ***
   E: control: grid structure                              [3.2.1]                      NO ***
   E: on-line control: 2*DT wave control point             [3.2.2]                      YES
   E: on-line control: standard deviations                 [3.2.2]                      YES
   E: on-line control: area averages                       [3.2.2]                      YES
   E: on-line control: constant mass                       [3.2.2]                      YES
```

```
   E: on-line control: valid range of values              [3.2.2]                      YES
   E: off-line control: 2*DX, 2*DY waves                  [3.2.3]                      YES
   E: off-line control: results independent from grid     [3.2.3]                      YES
   E: off-line control: comparison/plausible results      [3.2.3]                      NO ***
**********************************************************************************************
                         E V A L U A T I O N   R E S U L T :
**********************************************************************************************
The mesoscale model ZISCH (Version 2.00) is

*****   N O T   E V A L U A T E D   *****

in accordance with VDI guideline 3783 Sheet7 (Nov.2000).

I certify that all informations set out in this certificate are accurate and correct.
Statements regarding model properties are in accordance with those given by the model
developer (person responsible of model release, see point 0. above). No efforts have
been done to fit the model results to the reference data of test cases a to d.



-----------------------------           -----------------------------
(Place and Date)                        (Hans_Mustermann)
**********************************************************************************************
This evaluation certificate was created by program EVA (Version 1.0),
part of program METRAS+ (Version 1.0).
$$$$$$$$$$$$$$$$$$$$$$$$ EVA CERTIFICATION KEY: poqi80mxMwH9la#D#P9yafrp $$$$$$$$$$$$$$$$$$$$$$$
(It can be proved by this key that no modifications have been done to the certificate.)
**********************************************************************************************
```

Erläuterungen:

Der Abschnitt 0 enthält die Angaben zu Modell, Version und verantwortlichen Personen.

In den Abschnitten 1 und 2 wird aufgeführt, welche Anforderungen der Richtlinie an Dokumentation und Modelleigenschaften von dem Modell erfüllt werden.

Im Abschnitt 3 sind die Ergebnisse der Testfälle zusammengefasst. Das Evaluierungszertifikat enthält keine Trefferquoten oder andere Details zu den Testfällen mehr, sondern nur die Aussage, ob die Trefferquoten zu größer/gleich 2/3 („YES") oder kleiner als 2/3 („NO") berechnet wurden. Dies ist das ausschlaggebende Kriterium nach der Richtlinie. Außerdem sind im Abschnitt 3 die Aussagen zu Online- und Offlinekontrolle des Modells aufgelistet.

Es folgt die Gesamtbewertung des Evaluierungsprozesses. Im vorliegenden Fall ist das Modell nicht evaluiert. Sind alle notwendigen Kriterien, nicht aber unbedingt alle optionalen Kriterien erfüllt, so wird an dieser Stelle auf die vollständige Evaluierung und ggf. die Einschränkung des Anwendungsbereiches hingewiesen.

Abschließend erklärt die für die Evaluierung verantwortliche Person, dass alle Angaben im Zertifikat (ggf. nach den Angaben der für die Modellentwicklung verantwortlichen Person) wahrheitsgemäß sind und die in die Evaluierung eingeflossenen Modellergebnisse nicht nachträglich an die Referenzdaten angepasst worden sind. Das Zertifikat ist von der verantwortlichen Person zu unterschreiben.

Jedes Evaluierungszertifikat wird von EVA mit einem Schlüssel versehen, anhand dessen eine versehentliche Änderung des als ASCII-Datei auf dem Rechner abgelegten Zertifikats festgestellt werden kann.

Danksagung

Diese Arbeit wurde teilweise durch die "Bundesstiftung Umwelt" unter der Fördernummer 16839 finanziell unterstützt. Die Autoren sind für den Inhalt der Veröffentlichung verantwortlich.

Anhang A: Dateiformate und VDI-Kriterien

A.1 EVA-Modellergebnisdateien (*.efm) und Messdaten

Modellergebnisdateien im sogenannten EVA-Format bestehen grundsätzlich aus zwei *Kopfzeilen* und einer beliebigen Anzahl von *Datenblöcken*.

Beispiel für eine Modellergebnisdatei mit Kopfzeilen und 2 Datenblöcken:

```
'ZISCH'   '2.00'   'a'   'Hans_Mustermann'   '2001-07-30'
       1       20       1       20       1       35
###    49.8287888889     8.7358333333    10.0000000000     0.0000000000     1     1     1
       2        3
DD FF TP
99999999 03:00    1.0817942550    2.1107085850  287.0797670000
99999999 06:00    1.0850368850    2.1017103250  287.0797670000
###    49.8287888889     8.7358333333    30.0000000000     0.0000000000     1     1     2
       2        3
DD FF TP
99999999 03:00    1.3031714750    2.7233556450  287.0797670000
99999999 06:00    1.3072397450    2.7123867650  287.0797670000
```

Erläuterung

Zeile	Inhalt und Format
1. Kopfzeile	Modellname, Modellversion, Testfall, Benutzername und Modellrechnung jeweils als Zeichen in Hochkomma eingeschlossen. Kein festgelegtes Format.
2. Kopfzeile	Erster und letzter Gitterpunktindex in x-Richtung, erster und letzter Gitterpunktindex in y-Richtung, erster und letzter Gitterpunktindex in z-Richtung. Bei den Testfällen d1 und d2 sind diese Angaben überflüssig, die Zeile muss aber (ggf. als Leerzeile) in der Datei enthalten sein. FORTRAN-Format: (6(1X,I8))
1. Datenblockzeile	Die Kennung ### markiert den Beginn eines neuen Datenblocks. Es folgen geographische Länge und Breite [° dezimal, westl. Längen und südl. Breiten sind negativ anzugeben], Höhe des Gitterpunktes über Grund [m], Höhe der Orographie unterhalb des Gitterpunktes [m über NN] und Gitterpunktindizes i, j, k in x-, y- und z-Richtung. Bei den Testfällen d1 und d2 können Orographiehöhe und Gitterpunktindizes entfallen. FORTRAN-Format: (A3,4(1X,F16.10),3(1X,I8))
2. Datenblockzeile	Anzahl der in diesem Datenblock enthaltenen Zeitschritte und Vergleichsgrößen. FOTRAN-Format: (I8,1X,I8)
3. Datenblockzeile	Kennungen der in diesem Datenblock enthaltenen Vergleichsgrößen (siehe unter Schlüsselwort *X_nclass_KK* im Abschnitt 5.1.1). In den nachfolgenden Datenblockzeilen müssen die Werte der Vergleichsgrößen in der hier angegebenen Reihenfolge stehen. FORTRAN-Format: (n(A2,1X)) mit n: Anzahl der Kennungen

ab 4. Datenblockzeile	Pro Zeitschritt (siehe 2. Datenblockzeile) folgt je eine Datenblockzeile: Datum [yyyymmdd] und Uhrzeit [hh:mm] der Modellausgabe und je ein Wert pro Vergleichsgröße in der Reihenfolge, wie sie durch die 3. Datenblockzeile festgelegt ist. Sind Datum und/oder Uhrzeit irrelevant, wird „99999999“ bzw. „99:99“ angegeben. Für Vergleichgrößen mit nicht definiertem Wert ist „-999.“ anzugeben. FORTRAN-Format: (I8,1X,A5,n(1X,F15.10)) mit n: Anzahl der Vergleichsgrößen.

Die mit EVA ausgelieferten Messdatendateien (Referenzdatensätze der Testfälle d1 und d2) sind, abgesehen von drei kleinen Unterschieden, analog zu dem EVA-Format aufgebaut:

- Die 1. Kopfzeile enthält nur die vier Angaben Messkampagnenname, Testfall, Benutzername und Datum der Messdatenaufbereitung.
- Die 2. Kopfzeile ist leer bzw. kann für einen Kommentar verwendet werden.
- Die 1. Datenblockzeile endet nach den Koordinaten des Messpunktes.

A.2 Implementierte VDI Prüfkriterien

Die in der aktuellen EVA-Version implementierten Prüfkriterien (Tabellen A.2.1 bis A.2.8) entsprechen dem der (in Vorbereitung befindlichen) VDI Richtlinie 3783 Blatt 7, wie sie im November 2000 dem Entwurf der Richtlinie entnommen werden konnten. Soweit zukünftig Programmänderungen aufgrund des entgültigen Richtlinientextes erforderlich sind, werden diese im Rahmen einer neuen Versionsnummer implementiert.

Prüfkriterien Abschnitt 1 der VDI Richtlinie: Dokumentation
• Nachvollziehbarkeit • Kurzbeschreibung des Modells • Ausführliche Modellbeschreibung • Handbuch • Technische Referenz
Prüfkriterien Abschnitt 2 der VDI Richtlinie: Wissenschaftliche Bewertung
• Windkomponenten prognostisch • Temperatur prognostisch • spezifische Feuchte prognostisch • Kontinuitätsgleichung oder anelastische Approximation • Auftriebskräfte • Turbulenzparametrisierung stabilitätsabhängig • Corioliskraft • Flüsse stetig als Funktion des Ortes • Flüsse stetig als Funktion der Schichtung • oberflächennahe Flüsse direkt oder nach MO-Theorie berechnet • Symmetrie des Schubspannungstensors • Orographie explizit aufgelöst • Bewuchs und Bebauung über Rauhigkeitslänge • dreidimensional nicht äquidistantes Gitter • bodenfolgende Koordinaten • Wolkenmikrophysik • Eisphase • subskalige Konvektion • Bodenenergiebilanz mindestens „force-restore“ • Oberflächenfeuchtebilanz
Prüfkriterien Abschnitt 3 der VDI Richtlinie: Kontrolle der Modellrechnungen
• Gitterstruktur • 2*DT Wellen • Standardabweichungen • Gebietsmittelwerte • Massenerhaltung • Zulässigkeitsbereich der Modellergebnisse • 2*DX, 2*DY Wellen • gitterunabhängige Ergebnisse • Plausibilität

Tabelle A.2.1: Implementierte Prüfkriterien zu Modelleigenschaften

Vergleichsgröße	***Kürzel in EVA***	***Nachweisgrenze R_0***	***erlaubte Abweichung D_0***
Windrichtung	*DD*	*FF* > 1 m/s	0.1 °
Windgeschwindigkeit	*FF*	-	0.005 m/s
potentielle Temperatur	*TP*	-	10^{-6} K

Tabelle A.2.2: Implementierte Prüfkriterien zu Testfall a

Vergleichsgröße	***Kürzel in EVA***	***Nachweisgrenze R_0***	***erlaubte Abweichung D_0***
Windrichtung	*DD*	*FF* > 1 m/s	1 °
Windgeschwindigkeit	*FF*	-	0.05 m/s
potentielle Temperatur	*TP*	-	10^{-6} K

Tabelle A.2.3: Implementierte Prüfkriterien zu Testfall b1

Vergleichsgröße	***Kürzel in EVA***	***Nachweisgrenze R_0***	***erlaubte Abweichung D_0***
Windrichtung	*DD*	*FF* > 1 m/s	1 °
Windgeschwindigkeit	*FF*	-	0.05 m/s
potentielle Temperatur	*TP*	-	0.01 K

Tabelle A.2.4: Implementierte Prüfkriterien zu Testfall b2

Vergleichsgröße	***Kürzel in EVA***	***Nachweisgrenze R_0***	***erlaubte Abweichung D_0***
Windrichtung	*DD*	*FF* > 1 m/s	40 °
Windgeschwindigkeit	*FF*	-	1.5 m/s
Druck	*PP*	-	1.7 hPa
relative Feuchte	*RH*	-	10 % absolut
Realtemperatur	*TT*	-	2 K
Vertikalwind	*WW*	-	0.1 m/s

Tabelle A.2.5: Implementierte Prüfkriterien zu Testfall d1

Vergleichsgröße	***Kürzel in EVA***	***Nachweisgrenze R_0***	***erlaubte Abweichung D_0***
Windrichtung	*DD*	*FF* > 1 m/s	40 °
Windgeschwindigkeit	*FF*	-	1.5 m/s
Druck	*PP*	-	1.7 hPa
relative Feuchte	*RH*	-	10 % absolut
Realtemperatur	*TT*	-	2 K
Vertikalwind	*WW*	-	0.1 m/s

Tabelle A.2.6: Implementierte Prüfkriterien zu Testfall d2

Literatur

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[3] Bigalke, K., Schlünzen, K.H., Haenel, H.-D., Panskus H. (2001): Dokumentation des Modellsystems METRAS$^+$. *Meteorologisches Institut, Universität Hamburg, METRAS Technical Rep. 12-D*.

EVA (Version 1.0)

A Program for Evaluation of Mesoscale Models Following VDI Guideline 3783, Sheet 7

Program Documentation

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Contents

1. Introduction

The VDI Guideline 3783 Sheet 7 „Prognostic mesoscale non-hydrostatic wind field models – evaluation for dynamically and thermally induced flow fields“ [1] defines evaluation criteria for the quality assurance of mesoscale wind field models. Models that meet all evaluation criteria are classified as evaluated in accordance with this guideline. The evaluation of a model of a certain model version has to be recorded in the form of an evaluation protocol. This protocol can be used to show clients or authorities that the model evaluation was successful.

The program EVA is the technical implementation of the VDI guideline and facilitates the evaluation process for an arbitrary mesoscale model. The program accepts information via the input control. The EVA user gives information on necessary and optional model and application properties. Furthermore the user has to provide files with model results to seven test cases defined in the guideline. EVA checks all necessary test properties and calculates the hit rates of the model for each test case. Finally it creates an “Evaluation Certificate” (evaluation protocol), that can be printed and signed by the user. This certificate may be submitted to the clients resp. authorities.

METRAS PC [2] users have the advantage that EVA can read files with model results provided by METRAS PC without any previous conversion. EVA itself converts these files to the expected format.

EVA 1.0 is available as stand-alone version and also integrated into the program system **METRAS+** (Version 1.0) [3]. This documentation refers to both program versions. Sections that are not relevant for **METRAS+** are marked separately.

2. Evaluation Criteria of the Guideline

The evaluation guideline VDI 3783, Sheet 7 does not prescribe a certain model or fixed model properties, but defines rules for evaluation and minimum requirements the model has to meet. Below the basic concept of the guideline is summarised. The details are available in the guideline text [1].In this documentation they are only described[3] if it is necessary for understanding the program.

The evaluation criteria given in the VDI guideline are subdivided into three sections.

2.1. General Assessment

This sections contains requirements referring to the documentation of the model, to the comprehensibility and feasibility. Necessary criteria are (among other) publications in peer reviewed journals, the program documentation and how easy it is for a third party to test and verify both model and program.

2.2. Scientific Assessment

The scientific assessment is supposed to ensure that the model is based on the physical fundaments appropriate for the specified field of application. The requirements distinguish between essential criteria, which have to be met by the model, and optional criteria, that are only important for certain fields of application.

Essential criteria are (besides other criteria) the completeness of the set of equations, the validity of approximations and parameterisations. In contrast to that cloud microphysics is an

[3] The criteria implemented in the current program version are listed in Appendix A.2. Since the guideline 3783, Sheet 7 has not been finally accepted when the development of the program was finished, the final criteria may differ from those implemented in the program. The criteria correspond to the state of the guideline in November 2000.

optional criterion. It is only important if the formation of clouds has to be considered in a concrete model application.

2.3. Validation and Result Control

In the validation there are seven groups of test cases, which have to be successfully simulated by the model (Table 1). Twelve resp. 13 model calculations are necessary. Depending on the test case the results are compared to model results, analytic solutions or data from measuring campaigns. The assessment is conducted with the aid of hit rates. For a successful validation a hit rate of at least 2/3 has to be reached in each single test case. Permitted deviations between model results and reference data depend on the test case and are defined in the guideline.

Test case	Type of orography / land use	Tested properties	Changed parameter	No. of model simulations	Reference dataset
a	homogeneous terrain	numerical accuracy	wind direction	5	model result a1
b1	mountain ridge	influence of orography	-	1	analytic solution
b2	mountain ridge	influence of stratification and wind speed	wind speed	2	analytic solution
c1	idealised coast	ground temperature	-	1	plausibility check
c2[4]	idealised coast	condensation	-	1	Model result c1
d1	hill	complex orography influence	-	1	Dataset from measuring campaigns
d2	Berlin area	diurnal variation	-	1	Dataset from measuring campaigns

Table 1: Test cases of VDI 3783, Sheet 7

These seven groups of test cases are supposed to check single model properties in an isolated way. Numerical properties, orography effects, the influence of stability and the realistic consideration of real orography and land use are among these tested properties.

Further demands on the model are defined in a list of criteria for online and offline quality checks. Test criteria are the development of numerically induced waves, the mass conservation and properties of the used model grid.

2.4. Final assessment

The final assessment results from all evaluation criteria mentioned above. Based on all results of each single check the model user has to generate a compiling evaluation protocol. All evaluation criteria have to be listed and assigned to ”yes“ if the demands are met or to “no” if not. The model is evaluated in accordance with the guideline, if each model check was successful. If at least one demand was not met, the model is not successfully validated. The model is only valid for those applications that are covered by the criteria met by the model.

[4] *This test is optional and conducted only if the model should be able to represent cloud formation processes.*

3. Check of Test Cases in EVA

The user has to provide model result files in the EVA-input format (Section 5.1.2 and Appendix A.1) for each test case of the guideline. If the Model METRAS PC is to be evaluated, the user can also directly use the output files of the model. These are converted into the EVA-format by EVA. The evaluation is always done based on the files in the EVA-format. This procedure makes sure that METRAS PC is treated in the same way as other models and that hit rates are not changed because no temporal or spatial interpolation may be necessary.

The runtime protocol (Section 5.2.1) contains the analysis of the results of each test case together with the model properties (Section 5.1.1) given by the user. They are listed in detail in the protocol, while the evaluation certificate (Section 5.2.2) summarises them in accordance with the guideline.

The criteria of the VDI Guideline 3783 Sheet 7, used in the paragraphs of this chapter and implemented in the current program version of EVA can be found in Appendix A.2. Once again it should be mentioned that they correspond to the state of the guideline in November 2000.

3.1. Test Case a

This test case comprises five files containing model results. They are to be provided in the same order as there are listed in Table 2, which also gives information on the file content.

File-No.	Content
1	Reference case a1: wind direction 0°
2	Comparison case a2: wind direction 45°
3	Comparison case a3: wind direction 90°
4	Comparison case a4: wind direction 180°
5	Comparison case a5: wind direction 270°

Table 2: Model results test case a

The following criteria are checked resp. calculated by the program EVA in accordance with the guideline.

Grid Structure

- number of model grid points
- horizontal grid size Δx and Δy (tolerance: +/- 2 m)
- minimum vertical grid spacing Δz (tolerance: +/- 0.5 m)
- upper boundary of the model area at least 2500 m (tolerance: 0 m)

Time Increment Between Outputs

- time increment between two outputs (every 3 hours until 6 hours of model integration time).

Plausibility Check

- geographic co-ordinates, height and topography height defined at each read grid point?
- does each grid point occur only once in the input data?

Comparison of Input Files

- order and co-ordinates of the grid points identical to reference case a1?
- same time and time increment used as in the reference case?

Hit Rates

If all above criteria have been checked without any error, the hit rates[5] for the reference quantities defined in the guideline are calculated. Only those values are considered that exceed the validation limit. Every grid point is considered during this process.

3.2. Test Case b1

The following criteria are checked resp. calculated by the program EVA in accordance with the guideline.

Grid Structure

- number of model grid points
- horizontal grid size Δx and Δy (tolerance: +/- 2 m)
- minimum vertical grid size Δz (tolerance: +/- 0.5 m)
- upper boundary of the model area at least 2500 m (tolerance: 0 m)
- model topography (tolerance: +/- 0.1 m)

Time Increment Between Outputs

- time increment between two outputs (every 3 hours until 9 hours of model integration time).

Plausibility Check

- geographic co-ordinates, height and topography height defined at each read grid point?
- does each grid point occur only once in the input data?

Hit Rates

If all criteria above have been checked without any error, the hit rates[6] for the reference quantities defined in the guideline are calculated. Only those values are considered that exceed the validation limit. Only those grid points are considered that lie within the area that is supposed to be analysed, i.e. the area between 1000 m and 6000 m above sea level.

In the test case b1 the analytic Long-solution (see [1]) is used to calculate the reference data. Values of this solution are calculated at each read grid point, where the grid point co-ordinates are used.

3.3. Test Case b2

This test case consists of two files containing model results. They are provided in the same order as listed in Table 3, which also gives information about the file content.

File-No.	Contents
1	b2-1: geostrophic wind 10 m/s
2	b2-2: geostrophic wind 5 m/s

Table 3: Model result files for test case b2

The following criteria are checked resp. calculated by the program EVA in accordance with the guideline.

Grid Structure

[5] *Applied criteria see Table A.2.2.*

[6] *Applied criteria see Table A.2.3.*

- number of model grid points
- horizontal grid size Δx and Δy (tolerance: +/- 2 m)
- minimum vertical grid size Δz (tolerance: +/- 0.5 m)
- upper boundary of the model area at least 2500 m (tolerance: 0 m)
- model topography (tolerance: +/- 0.1 m)

Time Increment Between Outputs

- time increment between two outputs (every 3 hours until 9 hours of model integration time).

Plausibility Check

- geographic co-ordinates, height and topography height defined at each read grid point?
- does each grid point occur only once in the input data?

Hit Rates

If all above criteria have been checked without any error, the hit rates[7] for the reference quantities defined in the guideline are calculated. Only those values are considered that exceed the validation limit. Only those grid points are considered that lie within the area that is supposed to be analysed, i.e. the area between 1000 m and 6000 m above sea level.

In the test case b2 the analytic Long-solution (see [1]) is used to calculate the reference data. Values of this solution are calculated at each read grid point, where the grid point co-ordinates are used.

Wave Length

To calculate the vertical wave length out of the model results the x-z-cross section in the middle of the model area is considered. In this cross section the vertical column containing the maximum vertical wind speed is determined. Then all grid points within this column containing a local minimum or maximum of vertical wind speed are determined. Here all data in the column, from the surface to the model top are checked, the check is not restricted to the vertical area that is considered to calculate the hit rates. The wavelength results from the average of all height differences between the grid points of adjacent minima and maxima.

The hit rate for the point „wave length“ is 100%, if the wavelength calculated from the model results does not differ from the analytical solution more than 25% (see [1]). This percentage corresponds to the allowed deviation that is defined in the guideline. If the difference is greater than 25%, the hit rate is 0%.

3.4. Test case c1

The following criteria are checked resp. calculated by the program EVA in accordance with the guideline.

Grid Structure

- number of model grid points
- horizontal grid size Δx and Δy (tolerance: +/- 2 m)
- minimum vertical grid size Δz (tolerance: +/- 0.5 m)
- upper boundary of the model area at least 5000 m (tolerance: 0 m)

Time Increment Between Outputs

- time increment between two outputs (every 4 hours until 24 hours of model integration time).

[7] *Applied criteria see Table A.2.4.*

Plausibility Check

- geographic co-ordinates, height and topography height defined at each read grid point?
- does each grid point occur only once in the input data?

Hit Rates

If all above criteria have been checked without any error, the hit rate is calculated. For this test case the guideline only demands a comparison of the inland penetration of the sea breeze front for the time intervals 12-16LT and 16-20LT. If the inland penetration increases between both time intervals, the hit rate is 100%, otherwise it is 0%.

The position of the sea breeze front is estimated by EVA at the three output times 12, 16 and 20LT. It is estimated on the basis of four criteria:

1. location of the minimum divergence (=maximum convergence)
2. location of the maximum positive vertical velocity
3. location of the maximum potential temperature gradient in y-direction
4. location of the maximum gradient of relative humidity in y-direction

The positions determined are averaged thereby neglecting locations that deviate more than 4 km from the location determined by the minimum divergence criterion. Finally, the average penetration rates during the time intervals 12-16LT and 16-20LT are calculated from the averaged front positions.

3.5. Test Case c2

The following criteria are checked resp. calculated by the program EVA in accordance with the guideline.

Grid Structure

- number of model grid points
- horizontal grid size Δx and Δy (tolerance: +/- 2 m)
- minimum vertical grid size Δz (tolerance: +/- 0.5 m)
- upper boundary of the model area at least 5000 m (tolerance: 0 m)

Time Increment Between Outputs

- time increment between two outputs (every 4 hours to 24 hours of the model integration time).

Plausibility Check

- geographic co-ordinates, height and topography height defined at each read grid point?
- does each grid point occur only once in the input data?

Hit rates

If all above criteria have been checked without any error, the hit rate is calculated. Like in test case c1 the criterion is the inland penetration of the sea breeze front. It is calculated in the same way as in test case c1. Additionally, the penetration rate and the maximum vertical wind speed have to exceed the values of the corresponding time intervals of test case c1.

Because this comparison depents on the results of test case c1, test case c2 can only be evaluated by EVA, if test case c1 has been evaluated.

3.6. Test Cases d1 and d2

Test case d1 comprises two files containing model results. They are provided in the same order as listed in Table 4, which also gives information about the file content. For test case d2 only one model result file exists.

File-No.	Contents
1	d1-1: neutral stratification
2	d1-2: stable stratification

Table 4: Model result files for test case d1

The following criteria are checked resp. calculated by the program EVA in accordance with the guideline.

Structure and Content of the Model Result Files

The reference files containing the measured values of both test cases are delivered by EVA (files *d11.dat*, *d12.dat* and *d21.dat*; see Section 5.1.3). The user has to supply the model results in the same order as given in the comparison data, i.e. the order of the co-ordinates of the measurement points and the order of the quantities that are to be compared need to be the same. Where necessary the model results have to be interpolated to the location and time of the measurement points. If the structure of both files do not match, an evaluation of the test cases is impossible.

Hit Rates

If all above criteria have been checked without any error regarding structure and content, the hit rates[8] for the reference quantities defined in the guideline are calculated. Only those values are considered that exceed the validation limit.

4. Statistical Analysis

Apart from hit rates the VDI guideline does not demand further calculations of statistical quantities to point out the differences between model results and reference data (model results, analytic solution or measured data). However, in case that the model does not reach the necessary hit rates it is helpful for the user to get further information on deviations of the model results. Therefore, for the test cases a, b and d EVA calculates some statistical quantities regarding the differences between model results and reference data. For the test cases c this is not possible, because here the guideline does not demand a data comparison, but only a plausibility check.

During the statistical analysis as well as during the calculation of hit rates only those model results *M* and reference data *R* are considered that exceed the validation limit R_0[9]. For a given quantity data above the validation limit are available at *J* grid resp. reference points. For the statistical analysis and the calculation of hit rates all differences

$$D_j = \left| M_j - R_j \right| \quad j = 1, J$$

are considered. All data points with $D_j < D_0$ are treated as hit, where D_0 is the allowed deviation of the respective quantity.

The guideline only allows the two possibilities “hit rate >= 2/3“ or “hit rate < 2/3“ as result of the evaluation process. EVA also gives further information in the runtime protocol (Section 5.2.1).

[8] *Applied criteria see Table A.2.5, A.2.6.*

[9] *The validation limit is only for the wind direction not equal zero (see Appendix A.2).*

There the percentage of the hit rate is stated per quantity as well. Furthermore the mean difference

$$\overline{D} = \frac{1}{J}\sum_{j=1}^{J} D_j$$

and the root mean square error

$$RMSE = \sqrt{\frac{1}{J}\sum_{j=1}^{J} (D_j)^2}$$

are calculated from the differences and listed in the runtime protocol. If the model does not reach the necessary hit rate, further information on the maximum differences and on the frequency distribution of the differences is given. EVA calculates the minimum difference $\min(D_j)$, the maximum difference $\max(D_j)$, their location in geographical co-ordinates and their height, and finally date and time. Then the frequency distribution over N difference classes $n=0,N$ is determined. Within each class all differences D_j are counted that lie within the class boundary L_n:

$$L_{n-1} \le D_j < L_n$$

The number N and the class boundary L_N can be selected by the user, while each class boundary is determined by the program according to Table 5.

Class n	Lower boundary L_n	Upper boundary L_{n+1}
0	$-\infty$	*0*
1,...,N-1	$(n-1)*\frac{L_N}{N-1}$	$n*\frac{L_N}{N-1}$
N	L_N	$+\infty$

Table 5: Class limits for determining the frequency distribution of differences

Usually L_N should be set to the allowed deviation D_0. In this case all “hits“ belonging to the classes *1* to *N-1* are counted. A more detailed analysis of the “non-hits” is possible by choosing a value $L_N > D_0$.

By definition negative differences D_j are not permitted. For that reason class 0 contains all data points that are not defined resp. that are below the validation limit.

5. Files

5.1. EVA-Input Files

5.1.1. Control File

EVA is controlled by the file *eva.inp*[10] that must be stored in the run directory of EVA. The file is read in free format. These are the rules for the control file:

[10] *This file is not needed for the* ***METRAS****$^+$-version of EVA. In* ***METRAS****$^+$ the control data are provided via the input dialogue.*

- Within each line all characters following an exclamation mark are treated as comment and therefore ignored.
- Each input is defined by `KEY WORD = KEY VALUE`
- The key value is read from the first non-blank character following the key word and the equal sign (“=“). It ends with the last character before the next blank or exclamation mark (“!”).
- Each line can contain only one key word plus key value.
- The order of the input values within the control file is arbitrary.
- Key words and key values may be missing as far as they are irrelevant for the evaluation.

An interpreted example for key values is given below.

Example for an *eva.inp*:

```
!==============================================================================
!                EVA - Input Control File (eva.inp)
!==============================================================================
! Note: Lines starting with "!" are interpreted as comment lines.
!       Data lines must consist of KEY_WORD = KEY_VALUE.
!       KEY_VALUEs are read from the first non-blank character following "="
!       and end with the last character before the next blank or "!",
!       for example:
!       model_name      =  Model 1        (Result: "Model")
!       model_name      =  model !1       (Result: "model")
!       model_relperson = Jack the Ripper (Result: "Jack")
!       model_relperson = Jack_the_Ripper (Result: "Jack_the_Ripper")
!       model_version   = 2 .0            (Result: "2")
!       model_version   = 2.0             (Result: "2.0")
!       The sequence of data lines and comment lines is free.
!------------------------------------------------------------------------------
!Part 0: Information on the Mesoscale Model
!------------------------------------------------------------------------------
 proj_title      = evltst_1          ! titel of evaluation project
 proj_person     = Erika_Mustermann   ! person responsible for evaluation
 model_name      = ZISCH              ! name of model to be evaluated
 model_version   = 2.0                ! model version
 model_reldate   = 2001/07/31         ! model release date
 model_relperson = Hans_Mustermann    ! person responsible for model release
 model_supperson = Hans_Mustermann    ! person supporting model version
 eval_cert = D:\tmp\EVA\Results       ! Path to write evaluation certificate
 eval_rep  = D:\tmp\EVA\Reports       ! Path to write evaluation report
!------------------------------------------------------------------------------
!Part 1: General Assessment
!------------------------------------------------------------------------------
!
 doc_com         = yes                ! model comprehensible (yes/no)
 doc_short       = yes                ! short documentation (yes/no)
 doc_long        = yes                ! long documentation (yes/no)
 doc_man         = yes                ! user manual (yes/no)
 doc_tref        = no                 ! technical reference (yes/no)
!
!------------------------------------------------------------------------------
!Part 2: Scientific Assessment
!------------------------------------------------------------------------------
!
 prop_uvwprog    = yes                ! u,v,w wind prognostic (yes/no)
 prop_tprog      = yes                ! T prognostic (yes/no)
 prop_qprog      = yes                ! q prognostic (yes/no)
 prop_conti      = yes                ! continuity equ./anelast.approx. (yes/no)
 prop_bouy       = yes                ! bouyancy forces (yes/no)
 prop_turpar     = yes                ! turbulence f(stability) (yes/no)
 prop_coriolis   = yes                ! Coriolis force (yes/no)
 prop_flxloc     = yes                ! flux steady f(location) (yes/no)
 prop_flxstab    = yes                ! flux steady f(stability) (yes/no)
 prop_flxmo      = yes                ! direct surf.flux or MO-theory
 prop_fritens    = yes                ! symmetric friction tensor (yes/no)
 prop_exphgt     = yes                ! explicit terrain height (yes/no)
 prop_rough      = yes                ! veget./build. as roughness (yes/no)
 prop_3dnoequi   = yes                ! 3d non-uniform grid (yes/no)
 prop_etacoor    = yes                ! surf. follow. coord. (yes/no)
 prop_cloud      = yes                ! cloud physics (yes/no)
```

```
 prop_ice        = yes                ! ice phase (yes/no)
 prop_subconv    = yes                ! subscale convection (yes/no)
 prop_surtemp    = yes                ! sur.flux w. force restore (yes/no)
 prop_surrad     = yes                ! sur.flux w. radiation (yes/no)
 prop_surincl    = yes                ! sur.flux w. inclin. (yes/no)
 prop_surshad    = yes                ! sur.flux w. shading (yes/no)
 prop_surhumid   = yes                ! sur.humidity prognostic(yes/no)
!
!-------------------------------------------------------------------------------
!Part 3: Validation
!-------------------------------------------------------------------------------
! Control of results (VDI guideline chapter 3.2)
!
 ctrl_grid       = yes                ! contr. of grid structure (yes/no)
 ctrl_2dt        = yes                ! contr. of 2*DT waves (yes/no)
 ctrl_sdev       = yes                ! contr. of std.deviation (yes/no)
 ctrl_aravg      = yes                ! contr. of area average (yes/no)
 ctrl_mass       = yes                ! contr. of mass (yes/no)
 ctrl_range      = yes                ! contr of val. range of values (yes/no)
 ctrl_2dxy       = yes                ! contr. of 2*DX/DY waves (yes/no)
 ctrl_indep      = yes                ! contr. of ind. from grid (yes/no)
 ctrl_plaus      = yes                ! contr. of results (yes/no)
!-------------------------------------------------------------------------------
!Part 3a: Control of test case "a"
!-------------------------------------------------------------------------------
a_run = 2                             ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
a_file1 = D:\tmp\EVA\Results\a1.efm   ! 1. model result file (or conv.METRAS result)
a_file2 = D:\tmp\EVA\Results\a2.efm   ! 2. model result file (or conv.METRAS result)
a_file3 = D:\tmp\EVA\Results\a3.efm   ! 3. model result file (or conv.METRAS result)
a_file4 = D:\tmp\EVA\Results\a4.efm   ! 4. model result file (or conv.METRAS result)
a_file5 = D:\tmp\EVA\Results\a5.efm   ! 5. model result file (or conv.METRAS result)
a_nclass_dd = 10                      ! dd: number of histogram classes
a_lowbnd_dd = 0.1                     ! dd: lower boundary of a_nclass_dd
a_nclass_ff = 10                      ! vv: number of histogram classes
a_lowbnd_ff = 0.005                   ! vv: lower boundary of a_nclass_ff
a_nclass_tp = 10                      ! tp: number of histogram classes
a_lowbnd_tp = 1.e-6                   ! tp: lower boundary of a_nclass_tp
! key_values if a_run = 2:
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm ! 1. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm ! 2. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm ! 3. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm ! 4. METRAS result file
a_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm ! 5. METRAS result file
a_METturb   = 1                       ! 1=Luepkes/Schluenzen, 2=TKE
a_METcloud  = 0                       ! run without(=0)/with(=1) cloud physics
a_METtrace  = 0                       ! run without(=0)/with(>=1) no. of tracer
a_METntimes = 2                       ! number of output times (see a_METtimes)
a_METtimes  = 3.00                    ! 1. output time
a_METtimes  = 6.00                    ! 2. output time
!-------------------------------------------------------------------------------
!Part 3b1: Control of test case "b1"
!-------------------------------------------------------------------------------
b1_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
b1_file = D:\tmp\EVA\Results\b1.efm   ! model result file (or conv.METRAS result)
b1_nclass_dd = 10                     ! dd: number of histogram classes
b1_lowbnd_dd = 1.                     ! dd: lower boundary of b1_nclass_dd
b1_nclass_ff = 10                     ! vv: number of histogram classes
b1_lowbnd_ff = 0.05                   ! vv: lower boundary of b1_nclass_ff
b1_nclass_tp = 10                     ! tp: number of histogram classes
b1_lowbnd_tp = 1.e-6                  ! tp: lower boundary of b1_nclass_tp
! key_values if b1_run = 2:
b1_METfile = d:\tmp\METRAS\Results\AOutMVDI-b1_00000000-00090000.mfm ! METRAS result file
b1_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
b1_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
b1_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
b1_METntimes = 3                      ! number of output times (see b1_METtimes)
b1_METtimes  = 3.00                   ! 1. output time
b1_METtimes  = 6.00                   ! 2. output time
b1_METtimes  = 9.00                   ! 3. output time
!-------------------------------------------------------------------------------
!Part 3b2: Control of test case "b2"
!-------------------------------------------------------------------------------
b2_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
```

```
                                      ! 2=convert METRAS results and evaluate
b2_file1 = D:\tmp\EVA\Results\b21.efm ! 1. model result file (or conv.METRAS result)
b2_file1 = D:\tmp\EVA\Results\b22.efm ! 2. model result file (or conv.METRAS result)
b2_nclass_dd = 10                     ! dd: number of histogram classes
b2_lowbnd_dd = 1.                     ! dd: lower boundary of b2_nclass_dd
b2_nclass_ff = 10                     ! vv: number of histogram classes
b2_lowbnd_ff = 0.05                   ! vv: lower boundary of b2_nclass_ff
b2_nclass_tp = 10                     ! tp: number of histogram classes
b2_lowbnd_tp = 0.01                   ! tp: lower boundary of b2_nclass_tp
! key_values if b2_run = 2:
b2_METfile1 = d:\tmp\METRAS\results\AOutMVDI-b21_00000000-00090000.mfm ! 1. METRAS result file
b2_METfile2 = d:\tmp\METRAS\results\AOutMVDI-b21_00000000-00090000.mfm ! 2. METRAS result file
b2_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
b2_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
b2_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
b2_METntimes = 3                      ! number of output times (see b2_METtimes)
b2_METtimes  = 3.00                   ! 1. output time
b2_METtimes  = 6.00                   ! 2. output time
b2_METtimes  = 9.00                   ! 3. output time
!-------------------------------------------------------------------------------
!Part 3c1: Control of test case "c1"
!-------------------------------------------------------------------------------
c1_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
c1_file = D:\tmp\EVA\Results\c1.efm   ! model result file (or conv.METRAS result)
! key_values if c1_run = 2:
c1_METfile = d:\tmp\METRAS\Results\AOutMVDI-c1_00000000-01000000.mfm ! METRAS result file
c1_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
c1_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
c1_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
c1_METntimes = 3                      ! number of output times (see c1_METtimes)
c1_METtimes  = 12.00                  ! 1. output time
c1_METtimes  = 16.00                  ! 2. output time
c1_METtimes  = 20.00                  ! 3. output time
!-------------------------------------------------------------------------------
!Part 3c2: Control of test case "c2"
!-------------------------------------------------------------------------------
c2_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
c2_file = D:\tmp\EVA\Results\c2.efm   ! model result file (or conv.METRAS result)
! key_values if c2_run = 2:
c2_METfile = d:\tmp\METRAS\Results\AOutMVDI-c2_00000000-01000000.mfm ! METRAS result file
c2_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
c2_METcloud  = 1                      ! run without(=0)/with(=1) cloud physics
c2_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
c2_METntimes = 3                      ! number of output times (see c2_METtimes)
c2_METtimes  = 12.00                  ! 1. output time
c2_METtimes  = 16.00                  ! 2. output time
c2_METtimes  = 20.00                  ! 3. output time
!-------------------------------------------------------------------------------
!Part 3d1: Control of test case "d1"
!-------------------------------------------------------------------------------
d1_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
d1_file1 = D:\tmp\EVA\Results\d11.efm ! 1. model result file (or conv.METRAS result)
d1_file2 = D:\tmp\EVA\Results\d12.efm ! 2. model result file (or conv.METRAS result)
d1_nclass_dd = 10                     ! dd: number of histogram classes
d1_lowbnd_dd = 40.                    ! dd: lower boundary of d1_nclass_dd
d1_nclass_ff = 10                     ! vv: number of histogram classes
d1_lowbnd_ff = 1.5                    ! vv: lower boundary of d1_nclass_ff
d1_nclass_tt = 10                     ! tt: number of histogram classes
d1_lowbnd_tt = 2.                     ! tt: lower boundary of d1_nclass_tt
d1_nclass_rh = 10                     ! rh: number of histogram classes
d1_lowbnd_rh = 10.                    ! rh: lower boundary of d1_nclass_rh
d1_nclass_pp = 10                     ! pp: number of histogram classes
d1_lowbnd_pp = 1.7                    ! pp: lower boundary of d1_nclass_pp
! key_values if d1_run = 2:
d1_METfile1 = d:\tmp\METRAS\Results\AOutMVDI-d11_00140000-00170000.mfm ! 1. METRAS result file
d1_METfile2 = d:\tmp\METRAS\Results\AOutMVDI-d12_00140000-00170000.mfm ! 2. METRAS result file
d1_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
d1_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
d1_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
d1_METntimes = 3                      ! number of output times (see d1_METtimes)
d1_METtimes  = 15.00                  ! 1. output time
d1_METtimes  = 16.00                  ! 2. output time
```

```
d1_METtimes  = 17.00                  ! 3. output time
!-------------------------------------------------------------------------------
!Part 3d2: Control of test case "d2"
!-------------------------------------------------------------------------------
d2_run = 2                            ! 0=no evaluation
                                      ! 1=evaluation
                                      ! 2=convert METRAS results and evaluate
d2_file = D:\tmp\EVA\Results\d2.efm   ! model result file (or conv.METRAS result)
d2_nclass_dd = 10                     ! dd: number of histogram classes
d2_lowbnd_dd = 40.                    ! dd: lower boundary of d2_nclass_dd
d2_nclass_ff = 10                     ! ff: number of histogram classes
d2_lowbnd_ff = 1.5                    ! ff: lower boundary of d2_nclass_ff
d2_nclass_tt = 10                     ! tt: number of histogram classes
d2_lowbnd_tt = 2.                     ! tt: lower boundary of d2_nclass_tt
d2_nclass_rh = 10                     ! rh: number of histogram classes
d2_lowbnd_rh = 10.                    ! rh: lower boundary of d2_nclass_rh
d2_nclass_pp = 10                     ! pp: number of histogram classes
d2_lowbnd_pp = 1.7                    ! pp: lower boundary of d2_nclass_pp
! key_values if d2_run = 2:
d2_METfile = d:\tmp\METRAS\Results\AOutMVDI-d11_00140000-00170000.mfm ! METRAS result file
d2_METturb   = 1                      ! 1=Luepkes/Schluenzen, 2=TKE
d2_METcloud  = 0                      ! run without(=0)/with(=1) cloud physics
d2_METtrace  = 0                      ! run without(=0)/with(>=1) no. of tracer
d2_METntimes = 3                      ! number of output times (see d2_METtimes)
d2_METtimes  = 15.00                  ! 1. output time
d2_METtimes  = 16.00                  ! 2. output time
d2_METtimes  = 17.00                  ! 3. output time
!-------------------------------------------------------------------------------
```

Comments on the key words:

Key Word	***Comments***
	General information on the evaluation project:
proj_title	Title of the evaluation project
proj_person	Person responsible for the project
Model_name	Name of the model to be evaluated
Model_version	Version number of the model to be evaluated
Model_reldate	Model release date
Model_relperson	Person responsible for the model release
Model_supperson	Person supporting the model version
eval_cert	Path to write the evaluation certificate
eval_rep	Path to write the run protocol
	Model documentation as stated in Chapter 1 of the VDI guideline: *yes* (=is available resp. is true) or *no* (=is not available resp. is not true) are possible key values.
doc_com	Model is comprehensible for a third party
doc_short	Short model documentation
doc_long	Long model documentation
doc_man	User manual
doc_tref	Technical model reference
	Necessary model properties as stated in Chapter 2 of the VDI Guideline: *yes* (=is available resp. is true) or *no* (=is not available resp. is not true) are possible key values.
prop_uvwprog	Wind components prognostic
prop_tprog	Temperature prognostic
prop_qprog	Specific humidity prognostic
prop_conti	Continuity equation or anelastic approximation
prop_bouy	Buoyancy forces
prop_turpar	Parameterisation of turbulence is depending on stability
prop_coriolis	Coriolis force
prop_flxloc	Fluxes are steady functions of location
prop_flxstab	Fluxes are steady functions of stability
prop_flxmo	Direct calculation of surface fluxes / Monin-Obhukhov-Theory

prop_fritens	Symmetric friction tensor
prop_exphgt	Explicit terrain height
prop_rough	Vegetation / buildings as roughness length
prop_3dnoequi	Three dimensional non-uniform grid
prop_etacoor	Surface following co-ordinate system
prop_cloud	Cloud microphysics
prop_ice	Ice phase
prop_subconv	Subgrids scale convection
prop_surtemp	Surface fluxes with „force-restore“
prop_surrad	Surface energy budget with radiation
prop_surincl	Surface energy budget with inclination
prop_surshad	Surface energy budget with shading
prop_surhumid	Surface humidity budget equation
	Control of model results as stated in Chapter 3.2 of the VDI guideline: *yes* (=is available resp. is true) or *no* (=is not available resp. is not true) are possible key values.
ctrl_grid	Grid structure
ctrl_2dt	2*DT waves
ctrl_sdev	Standard deviation
ctrl_aravg	Area average
ctrl_mass	Mass conservation
ctrl_range	Validity range (plausible values)
ctrl_2dxy	2*DX, 2*DY waves
ctrl_indep	Results independent of grid
ctrl_plaus	Control of results
	Test cases a to d as stated in Chapter 3.1.1 of the VDI guideline: Depending on the test case the wildcards in the key words must be replaced as follows: *X*: symbol of the test case (*a, b1, b2, c1, c2, d1* or *d2*) *N*: number of files (a:*5*, b2:*2*, d1:*2*, *N* is not needed in the other cases) *KK*: Symbol for quantities that are to compare. Necessary quantities are listed for each test case in Appendix A.2. In EVA *KK* is generally replaced by: *DD*: wind direction *FF*: wind speed *UU*: u-wind component *VV*: v-wind component *WW*: w-wind component (vertical wind) *DV*: divergence *TP*: potential temperature *TT*: real temperature *RH*: relative humidity *PP*: pressure
*X*_run	= 0: no evaluation of this test case = 1: evaluation = 2: conversion of METRAS PC input files and evaluation
	The following key values must be stated only if *X*_run was set to a value greater than 0:
*X*_file*N*	Path and name of model result files. If the conversion of METRAS PC files is selected, the converted data are written to these files.
*X*_nclass_*KK*	Number of histogram classes for the statistical analysis (not for test cases c1, c2)
*X*_lowbnd_*KK*	Lower boundary of the last class (not for test cases c1, c2)
	The following key values have to be stated only if METRAS PC files shall be converted (*X*_run=2):

*X*_METfile*N*	Path and name of the METRAS PC result files
*X*_METturb	Parameterisation of turbulence used during the simulation = 1: Lüpkes/Schlünzen = 2: TKE
*X*_METcloud	Simulation run with (=0) or without (=1) cloud physics
*X*_METtrace	Simulation run with (=0) or without (=1) tracers
*X*_METntimes	Number of output times to be evaluated (must be identical to the demands of the guideline, independent of the number of output times available in the files)
*X*_METtimes	*X*_METtimes output times to be evaluated. For each output time one line is necessary.

5.1.2. Model result files

How many and which model result files have to be provided during an EVA calculation depends on the key value *X*_run in the control file[11].

Result files of models other than METRAS PC must be available in the EVA-file format that is explained in Appendix A.1. Especially for the test cases d1 and d2 it is important that not only demands on the file format are met, but also that the measurement points and measurement times are in the same order (see Section 3.6) as in the files containing the reference data (Section 5.1.3).

Result files[12] of METRAS PC [2]do not need to be prepared for EVA. EVA itself converts them into the required format. If the file has already been converted during an earlier EVA-calculation, a further conversion is not necessary.

5.1.3. Measured Data of the test cases d1 and d2

The VDI Guideline 3783 Sheet 7 defines reference datasets (measured data) for the test cases d1 and d2. These datasets are delivered with EVA and in case of successful installation they can be found in the installation directory *dat_meas* under the file name

- *d11.dat* 1st Reference dataset for test case d1 (neutral stratification)
- *d12.dat* 2nd Reference dataset for test case d1 (stable stratification)
- *d21.dat* Reference dataset for test case d2

They are readable ASCII-files in the EVA-format as described in Appendix A.1. Each time EVA is started these files are tested on authenticity. If the user changes and saves the file accidentally while viewing it, EVA has to be reinstalled.

5.2. EVA-Output Files

5.2.1. Runtime Protocol

Each EVA calculation generates a runtime protocol that is saved in the run directory under the name eva.*erp*[13]. In this file the control data are listed and all essential work steps of the program are documented. Additionally, it contains the results of the statistical analysis for the test cases a, b and d (Section 4).

---

[11] *In the **METRAS**+-version of EVA dependent on the corresponding values in the input dialogue.*

[12] *In the **METRAS**+-version of METRAS PC these files are saved with the default file extension *.mfm.*

[13] *In the **METRAS**+-version the protocol is saved under a different file name and partly contains different entries.*

Example for a runtime protocol:

```
****** EVA started at 2001-07-30 21:27:58
       ----------------------------------------
       | Meaning of following messages:       |
       | I#nnn:         info  message no. nnn |
       | W#nnn: warning error message no. nnn |
       | F#nnn: fatal   error message no. nnn |
       ----------------------------------------
I#100: ====================================================================
       !     ***** Control data of this evaluation project: *****         !
       !                                                                  !
       ! -----------------------------------------------------------------
       ! 1. General Information
       ! -----------------------------------------------------------------
       ! Evaluation project             = evltst_2
       ! Person responsible             = Erika_Mustermann
       ! Model name                     = METRAS_PC
       ! Model version                  = 2.00Beta
       ! Model release date             = 2001/07/31
       ! Person responsible for release = Hans_Mustermann
       ! Person responsible for support = Hans_Mustermann
       ! File with Evaluation Certificate:
       !  --> d:\tmp\EVA\Results\evltst_2.ece
       ! File with Evaluation Report:
       !  --> d:\tmp\EVA\Reports\evltst_2.erp
       ! -----------------------------------------------------------------
       ! 2.a Properties of model to be evaluated: Documentation
       ! -----------------------------------------------------------------
       ! Model comprehensible ........................... = YES
       ! Documentation, short version ................... = YES
       ! Documentation, long version .................... = YES
       ! User manual .................................... = YES
       ! Technical reference ............................ = YES
       ! -----------------------------------------------------------------
       ! 2.b Properties of model to be evaluated: Implementation
       ! -----------------------------------------------------------------
       ! Three wind components prognostic ............... = YES
       ! Temperature prognostic ......................... = YES
       ! Specific humidity prognostic ................... = YES
       ! Continuity equation or anelstic approximation ... = YES
       ! Buoyancy forces (eg. Boussinesq approximation) .. = YES
       ! Turbulence parameterization function of stability = YES
       ! Coriolis force ................................. = YES
       ! Fluxes steady (function of location) ........... = YES
       ! Fluxes steady (function of stability) .......... = YES
       ! Direct calculation of surface fluxes or MO theory = YES
       ! Symmetric friction tensor ...................... = YES
       ! Explicit elevation heights ..................... = YES
       ! Canopy/buildings as roughness lengths .......... = YES
       ! 3d non-equidistant grid ........................ = YES
       ! Surface following coordinates .................. = YES
       ! Cloud physic / short & longwave radiation ....... = YES
       ! Ice phase prognostic ........................... = YES
       ! Parameterization of subgrid scale convection ......... = YES
       ! Surface temperature at least with force restore = YES
       ! Surface fluxes with short & longwave radiation .. = YES
       ! Surface fluxes with surface inclination ......... = YES
       ! Surface fluxes with shading .................. = YES
       ! Surface humidity balance ....................... = YES
       ! -----------------------------------------------------------------
       ! 2.c Properties of model to be evaluated: Result Control
       ! -----------------------------------------------------------------
       ! Grid structure ................................. = YES
       ! On-line control: 2*DT waves .................... = YES
       ! On-line control: standard deviations ........... = YES
       ! On-line control: area averages ................. = YES
       ! On-line control: constant mass ................. = YES
       ! On-line control: valid ranges .................. = YES
       ! Off-line control: 2*DX & 2*DY waves ............ = YES
       ! Off-line control: result independent from grid .. = YES
       ! Off-line control: comparison / plausible results  = YES
       ! -----------------------------------------------------------------
       ! 3. Control of test case "a"
       ! -----------------------------------------------------------------
       ! Test case "a" selected for evaluation
       ! Conversion of METRAS result files to EVA format:
       !  --> D:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm
```

```
       !  --> D:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm
       !  --> D:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm
       !  --> D:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm
       !  --> D:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm
       ! Parameters of METRAS result file(s):
       !  turbulence parameterization = Luepkes/Schluenzen
       !  run with cloud physics      = NO
       !  number of tracer            =  0
       !  number of conversion times  =  2
       !  conversion time no.  1      =   3.000000
       !  conversion time no.  2      =   6.000000
       ! Model result file(s) in EVA format:
       ! (Result of METRAS file conversion)
       !  --> D:\tmp\EVA\Results\VDI-a11
       !  --> D:\tmp\EVA\Results\VDI-a12
       !  --> D:\tmp\EVA\Results\VDI-a13
       !  --> D:\tmp\EVA\Results\VDI-a14
       !  --> D:\tmp\EVA\Results\VDI-a15
       ! Classes defined for statistical analysis:
       ! (Note: Whatever is listed here - statistical analysis is done
       !        for those meteorological quantities only, which are part
       !        of the evaluation process. However, statistical analysis
       !        is NO part of the evaluation process but for user
       !        information and error analysis!)
       ! Key - no.of classes - lower boundary of highest class
       ! DD    10                   0.100000000000
       ! FF    10                   0.005000000000
       ! TP    10                   0.000001000000
       ! -------------------------------------------------------------------
       ! 4. Control of test case "b1"
       ! -------------------------------------------------------------------
       ! Test case "b1" not selected for evaluation
       ! -------------------------------------------------------------------
       ! 5. Control of test case "b2"
       ! -------------------------------------------------------------------
       ! Test case "b2" not selected for evaluation
       ! -------------------------------------------------------------------
       ! 6. Control of test case "c1"
       ! -------------------------------------------------------------------
       ! Test case "c1" not selected for evaluation
       ! -------------------------------------------------------------------
       ! 7. Control of test case "c2"
       ! -------------------------------------------------------------------
       ! Test case "c2" not selected for evaluation
       ! -------------------------------------------------------------------
       ! 8. Control of test case "d1"
       ! -------------------------------------------------------------------
       ! Test case "d1" not selected for evaluation
       ! -------------------------------------------------------------------
       ! 9. Control of test case "d2"
       ! -------------------------------------------------------------------
       ! Test case "d2" not selected for evaluation
I#101: !                                                                   !
       !   ***** End of control data of this evaluation project *****      !
       =====================================================================
I#204: $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
       $                                 $
       $ Start processing test case "a " $
       $                                 $
       $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a11
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a1_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a11
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm
I#107: Open output file:
```

```
       D:\tmp\EVA\Results\VDI-a12
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a2_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a12
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a13
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a3_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a13
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a14
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a4_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a14
I#206: ===== METRAS data conversion completed
I#205: >>>>> Convert METRAS results for evaluation.
             Details of conversion can be found in file "RMD.tmp"
             which is overwritten with each conversion.
I#105: File with model results or measurement data opened:
       D:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm
I#107: Open output file:
       D:\tmp\EVA\Results\VDI-a15
I#111: File reading completed for file:
       D:\tmp\METRAS\Results\AOutMVDI-a5_00000000-00060000.mfm
I#112: Writing to file completed for file:
       D:\tmp\EVA\Results\VDI-a15
I#206: ===== METRAS data conversion completed
I#207: >>>>> Rearrange data for statistical evaluation.
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a11
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a12
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a13
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a14
I#105: File with model results or measurement data opened:
       D:\tmp\EVA\Results\VDI-a15
I#107: Open output file:
       a.cdd
I#107: Open output file:
       a.cff
I#107: Open output file:
       a.ctp
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a11
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a11
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a12
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a12
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a13
I#109: EOF found after 98002 line(s) in file:
```

```
       D:\tmp\EVA\Results\VDI-a13
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a14
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a14
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#230: >>>>> Scan grid point coordinates in file:
       D:\tmp\EVA\Results\VDI-a15
I#109: EOF found after 98002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a15
I#130: Model data / Geogr. latitude: defined at all points.
I#130: Model data / Geogr. longitude: defined at all points.
I#130: Model data / Height z: defined at all points.
I#130: Model data / elevation height z_s: defined at all points.
I#231: >>>>> Start checking model grid
       Horizontal grid spacing in x-direction:
         Minimum Delta-x (m)     :  1999.485360236082
            (Number of occurences:  1 ;
            first occurence      :  ix,ix+1,iy = 10 11 15 )
         Maximum Delta-x (m)     :  1999.835902171675
            (Number of occurences:  1 ;
            first occurence      :  ix,ix+1,iy = 10 11 14 )
       Horizontal grid spacing in y-direction:
         Minimum Delta-y (m)     :  1999.803937169723
            (Number of occurences:  2 ;
            first occurence      :  ix,iy,iy+1 = 10 1 2 )
         Maximum Delta-y (m)     :  2000.237746986561
            (Number of occurences:  2 ;
            first occurence      :  ix,iy,iy+1 = 3 19 20 )
       Vertical grid spacing:
         Minimum Delta-z (m)     :  20.00000000000000
            (Number of occurences:  2000 ;
            first occurence      :  ix,iy,iz,iz+1 = 1 1 1 2 )
         Maximum Delta-z (m)     :  500.0000000000000
            (Number of occurences:  4400 ;
            first occurence      :  ix,iy,iz,iz+1 = 1 1 24 25 )
         I N F O:
         Maximum of vertical extent of model
         simulation domain as estimated by
         z(k_max)+0.5*[z(k_max)-z(k_max-1)]=  8674.000000000000  m
         satisfies value ( 2500.000000000000  m) required
         by the guideline.
         (Note: z(k) is height above ground.)
I#232: ===== Checking model grid completed successfully.
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a11
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a12
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a13
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a14
I#109: EOF found after 70002 line(s) in file:
       D:\tmp\EVA\Results\VDI-a15
I#113: Writing to converted-data files completed.
I#130: Model data / ff-values: defined at all points for all times.
I#130: Model data / dd-values: defined at all points for all times.
I#130: Model data / tp-values: defined at all points for all times.
I#208: ===== Data conversion completed.
I#210: >>>>> Start statistical evaluation.

       ***************************************************
       ***** Start evaluating "Wind direction (°)"
       ***************************************************

       Allowed deviation:  0.1000000000000000
       Width of classes:  1.111111111111111E-02

       Frequency Distribution of Differences
       - - - - - - - - - - - - - - - - - - -
       class           sum of
```

```
index   counts   counts   relsum(%)    class boundaries [lower/upper)
---------------------------------------------------------------------
   00        0        0      0.00 -999.000000000000    0.000000000000 (undefined)
---------------------------------------------------------------------
   01    55200    55200     75.00    0.000000000000    0.011111111111 )
   02        0    55200      0.00    0.011111111111    0.022222222222 )
   03        0    55200      0.00    0.022222222222    0.033333333333 )
   04     8800    64000     11.96    0.033333333333    0.044444444444 )
   05     7600    71600     10.33    0.044444444444    0.055555555556 ) within
   06      400    72000      0.54    0.055555555556    0.066666666667 ) criterion
   07        0    72000      0.00    0.066666666667    0.077777777778 )
   08        0    72000      0.00    0.077777777778    0.088888888889 )
   09        0    72000      0.00    0.088888888889    0.100000000000 )
---------------------------------------------------------------------
   10     1600    73600      2.17    0.100000000000 9999.000000000000 (above criterion)
---------------------------------------------------------------------
minimum difference      :    0.0000000000
maximum difference      :    0.1259011225
  -> at lat,lon,z       :         49.99070          9.26505        683.00000
  -> value at lat,lon,z :  359.8672847926
  -> at date            :        99999999
  -> at output time     :           06:00
mean difference         :    0.0127234826
rmse                    :    0.0275433350

++ Hit rate for currently processed quantity : 97.82608695652173  %
   (number of hits : total number of defined cases = 72000 : 73600 )

!! Overall hit rate after evaluating "DD": 97.826 %

***************************************************
***** Start evaluating "Wind speed (m/s)"
***************************************************

Allowed deviation:  5.000000000000000E-03
Width of classes:  5.555555555555556E-04

Frequency Distribution of Differences
- - - - - - - - - - - - - - - - - - -
class           sum of
index   counts   counts   relsum(%)    class boundaries [lower/upper)
---------------------------------------------------------------------
   00        0        0      0.00 -999.000000000000    0.000000000000 (undefined)
---------------------------------------------------------------------
   01    55200    55200     75.00    0.000000000000    0.000555555556 )
   02        0    55200      0.00    0.000555555556    0.001111111111 )
   03     1600    56800      2.17    0.001111111111    0.001666666667 )
   04     4400    61200      5.98    0.001666666667    0.002222222222 )
   05     3200    64400      4.35    0.002222222222    0.002777777778 ) within
   06     6000    70400      8.15    0.002777777778    0.003333333333 ) criterion
   07      800    71200      1.09    0.003333333333    0.003888888889 )
   08     1600    72800      2.17    0.003888888889    0.004444444444 )
   09        0    72800      0.00    0.004444444444    0.005000000000 )
---------------------------------------------------------------------
   10      800    73600      1.09    0.005000000000 9999.000000000000 (above criterion)
---------------------------------------------------------------------
minimum difference      :    0.0000000000
maximum difference      :    0.0073550356
  -> at lat,lon,z       :         50.00899          9.01396        819.50000
  -> value at lat,lon,z :    4.9961732872
  -> at date            :        99999999
  -> at output time     :           06:00
mean difference         :    0.0007138812
rmse                    :    0.0015360527

++ Hit rate for currently processed quantity : 98.91304347826087  %
   (number of hits : total number of defined cases = 72800 : 73600 )

!! Overall hit rate after evaluating "FF": 97.826 %

***************************************************
***** Start evaluating "Potential temperature (K)"
***************************************************

Allowed deviation:  1.000000000000000E-06
Width of classes:  1.111111111111111E-07

Frequency Distribution of Differences
```

```
- - - - - - - - - - - - - - - - - - - -
class          sum of
index   counts   counts   relsum(%)    class boundaries [lower/upper)
---------------------------------------------------------------------
   00        0        0      0.00 -999.000000000000    0.000000000000 (undefined)
---------------------------------------------------------------------
   01    73600    73600    100.00    0.000000000000    0.000000111111 )
   02        0    73600      0.00    0.000000111111    0.000000222222 )
   03        0    73600      0.00    0.000000222222    0.000000333333 )
   04        0    73600      0.00    0.000000333333    0.000000444444 )
   05        0    73600      0.00    0.000000444444    0.000000555556 ) within
   06        0    73600      0.00    0.000000555556    0.000000666667 ) criterion
   07        0    73600      0.00    0.000000666667    0.000000777778 )
   08        0    73600      0.00    0.000000777778    0.000000888889 )
   09        0    73600      0.00    0.000000888889    0.000001000000 )
---------------------------------------------------------------------
   10        0    73600      0.00    0.000001000000 9999.000000000000 (above criterion)
---------------------------------------------------------------------
minimum difference      :    0.0000000000
maximum difference      :    0.0000000000
  -> at lat,lon,z       :       -999.00000       -999.00000       -999.00000
  -> value at lat,lon,z : -999.0000000000
  -> at date            :            -999
  -> at output time     :            -999
mean difference         :    0.0000000000
rmse                    :    0.0000000000

++ Hit rate for currently processed quantity : 100.0000000000000  %
   (number of hits : total number of defined cases = 73600 : 73600 )

!! Overall hit rate after evaluating "TP": 97.826 %

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ Test case a (VDI-Guideline) - Overall hit rate :  97.826 % $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

       ===== Statistical evaluation completed (a).
I#211: ===== Statistical evaluation completed.
I#216: 0 warning errors detected.
I#999: Execution completed. No fatal error detected.
****** EVA completed at 2001-07-30 21:30:50
```

Comments:

Message number	Comment
I#100 / I#101	List of the input data.
I#204	Processing of a test case has started
I#205	Conversion of a METRAS PC output file to the EVA-format starts. During the conversion a temporal file *RMD.tmp* is created in the run directory. If there are any problems during the conversion, the file gives hints on failure causes. This file is overwritten during each conversion.
I#105	METRAS PC output file opened.
I#107	Conversion file opened.
I#111	Reading METRAS PC output file is completed.
I#112	Writing to conversion file is completed.
I#206	Conversion of the METRAS PC output file is completed.
I#207	To calculate the hit rates temporal files are created, in which the reference and model data are re-arranged.
I#105	Model result files (EVA-format) are opened and read
I#107	For each quantity that is compared a temporal file is created.
I#230	The grid co-ordinates of a model result file (EVA-format) are checked.
I#109	Reading is finished, grid co-ordinates have been checked.
I#130	Geographic co-ordinates, height and topography height are defined at all grid points.
I#231	The grid structure of all model result files is checked for agreement with the demands stated in the guideline: Report on the minimum and maximum grid spacing found and their location in the grid. Small deviations in comparison to the values used in

	the model may result from rounding errors and model output formats.
I#232	Checking model grid is successfully completed.
I#109	Reading for checking the grid structure is completed.
I#113	Writing to temporal files is completed.
I#130	Quantities defined at all points for all times.
I#208	Sorting reference and model data to temporal files is completed.
I#210	Output of hit rates and results of the statistical analysis for the current test case. For each quantity the following information is given: - the allowed deviation (in accordance with the guideline) of the quantity from the reference data and the width of classes (selected by the user) for the histogram of differences - the histogram of absolute differences between model and reference data. Within each class the number of grid points, their percentage and the class boundaries are stated. Class 0 contains all non-defined data points; (in the example) the highest class contains all points that do not lie within the allowed deviation. - minimum and maximum absolute difference and their location - mean absolute difference and root mean square error - hit rate for this quantity - overall hit rate after the calculation of the current quantity. The overall hit rate is always the minimum of all quantities that have been calculated so far.
I#211	Calculation of hit rates and statistical analysis are completed..
I#216 / I#999	No warnings or fatal errors were detected.

5.2.2. Evaluation Certificate

After a successful calculation by the program EVA an evaluation certificate is created. Its file name is made up by the project title (proj_title) and an extension „.ece“. The evaluation certificate is also created, if not all criteria of the guideline are satisfied. It can be printed, signed and then supplied to clients and authorities to prove that the mesoscale model was evaluated in accordance with the VDI Guideline 3783 Sheet 7.

Example for an Evaluation Certificate:

```
==============================================================================================
            Model Evaluation Certificate in Accordance with VDI Guideline 3783 Sheet7
==============================================================================================
This document certifies the evaluation of a prognostic mesoscale non-hydostatic wind field
model for dynamically and thermally driven wind fields. The certificate is in accordance with
VDI guideline 3783 Sheet7 (Nov.2000). Numbers in brackets [...] denote the corresponding
section of the guideline. Essential qualities are denoted "E", application dependent
qualities with "A".

----------------------------------------------------------------------------------------------
0. Information on the Mesoscale Model:
----------------------------------------------------------------------------------------------
   Name................................: ZISCH
   Version.............................: 2.00
   Release Date........................: 2001/07/31
   Responsible Person..................: Erika_Mustermann
   Responsible Person for this Evaluation: Hans_Mustermann
1. General Assessment:                                    [guideline]                 PASSED
----------------------------------------------------------------------------------------------
   E: Comprehensibility                                   [1.1]                       YES
   E: Documentation, short version                        [1.2.1]                     YES
   E: Documentation, long version                         [1.2.2]                     YES
   E: User Manual                                         [1.2.3]                     YES
   A: Technical Reference                                 [1.2.4]                     NO ***
----------------------------------------------------------------------------------------------
2. Scientific Assessment:                                 [guideline]                 PASSED
----------------------------------------------------------------------------------------------
   E: three wind components prognostic                    [2]                         NO ***
   E: temperature prognostic                              [2]                         YES
   E: specific humidity prognostic                        [2]                         YES
   E: continuity equation or anelastic approximation      [2]                         YES
   E: buoyancy forces (eg. Boussinesq approx.)            [2]                         YES
```

```
   E: turbulence parameterization function of stability   [2]                        YES
   E: Coriolis force considered                           [2]                        YES
   E: fluxes steady as function of location               [2]                        YES
   E: fluxes steady as function of stability              [2]                        YES
   E: direct calc. of surfaces fluxes or MO-theory        [2]                        YES
   E: symmetry of friction tensor                         [2]                        YES
   E: orography explicitly considered                     [2]                        YES
   E: vegetation and buildings as roughness lengths       [2]                        YES
   E: 3d non-uniform grid                                 [2]                        NO ***
   A: surface following coordinates                       [2]                        NO ***
   A: cloud physics / short and longwave radiation        [2]                        YES
   A: ice phase prognostic                                [2]                        YES
   A: parameterization of sub-grid scale convection       [2]                        YES
   A: surface temperature prognostic                      [2]                        YES
   A: surface fluxes with short and lonwave radiation     [2]                        YES
   A: surface fluxes with surface inclination             [2]                        YES
   A: surface fluxes with shading by mountains            [2]                        YES
   A: surface humidity prognostic                         [2]                        NO ***
--------------------------------------------------------------------------------------------
3. Validation:                                            [guideline]                PASSED
--------------------------------------------------------------------------------------------
   E: test case a -homogenous terrain                     [3.1.1]                    NO ***
   E: test case b1-mountain ridge/eff. of surface shape   [3.1.1]                    NO ***
   E: test case b2-mountain ridge/eff. of wind speed      [3.1.1]                    NO ***
   E: test case c1-idealized coast/eff. of surf. temp.    [3.1.1]                    NO ***
   E: test case c2-idealized coast/effect of clouds       [3.1.1]                    NO ***
   E: test case d1-field campaign Sophienhoehe            [3.1.1]                    NO ***
   E: test case d2-field campaign Berlin                  [3.1.1]                    NO ***
   E: control: grid structure                             [3.2.1]                    NO ***
   E: on-line control: 2*DT wave control point            [3.2.2]                    YES
   E: on-line control: standard deviations                [3.2.2]                    YES
   E: on-line control: area averages                      [3.2.2]                    YES
   E: on-line control: constant mass                      [3.2.2]                    YES
   E: on-line control: valid range of values              [3.2.2]                    YES
   E: off-line control: 2*DX, 2*DY waves                  [3.2.3]                    YES
   E: off-line control: results independent from grid    [3.2.3]                    YES
   E: off-line control: comparison/plausible results      [3.2.3]                    NO ***
********************************************************************************************
                         E V A L U A T I O N   R E S U L T :
********************************************************************************************
The mesoscale model ZISCH (Version 2.00) is

*****   N O T   E V A L U A T E D   *****

in accordance with VDI guideline 3783 Sheet7 (Nov.2000).

I certify that all informations set out in this certificate are accurate and correct.
Statements regarding model properties are in accordance with those given by the model
developer (person responsible of model release, see point 0. above). No efforts have
been done to fit the model results to the reference data of test cases a to d.



----------------------------        ----------------------------
(Place and Date)                    (Hans_Mustermann)
********************************************************************************************
This evaluation certificate was created by program EVA (Version 1.0),
part of program METRAS+ (Version 1.0).
$$$$$$$$$$$$$$$$$$$$$$$ EVA CERTIFICATION KEY: poqi80mxMwH9la#D#P9yafrp $$$$$$$$$$$$$$$$$$$$$$
(It can be proved by this key that no modifications have been done to the certificate.)
********************************************************************************************
```

Comments:

The section 0 contains information on the model, version and responsible persons.

In the Sections 1 and 2 it is stated which demands of the guideline on documentation and model properties are met by the model.

In Section 3 the results of the test cases are summarised. The evaluation certificate does not contain hit rates or other details on the test cases, but only the statement on the hit rate greater or equal to 2/3 („YES") or less than 2/3 („NO"). This is the decisive criterion in accordance with the guideline. Furthermore, information on online and offline control of the model is listed in Section 3.

It follows the overall assessment of the evaluation process. In our example the model is not evaluated. If all necessary, but not necessarily all optional criteria are satisfied, the complete evaluation and a possible restriction of the application area is indicated here.

Finally, the person responsible for the evaluation certifies that all information set out in the certificate is correct (where necessary according to information from the model developer) and that no efforts have been made to fit the model results to the reference data. The certificate has to be signed by the responsible person.

For each evaluation certificate an evaluation key is created. This key allows to detect an inadvertent change of the certificate, which is written to an ASCII file on the computer.

Acknowledgements

We thank Guido Schröder from the Meteorological Institute, University of Hamburg, for helping with the English version of this documentation.

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Appendix A: File Formats and VDI-Criteria

A.1 EVA-Model Result Files (*.efm) and Measured Data

Model result file in the so called EVA-format strictly consist of two *headers* and an arbitrary number of *data blocks*.

Example for a Model Result File Containing Header and 2 Data Blocks:

```
'ZISCH'   '2.00'   'a'   'Hans_Mustermann'   '2001-07-30'
       1       20       1       20       1       35
###    49.8287888889     8.7358333333    10.0000000000     0.0000000000     1     1     1
       2        3
DD FF TP
99999999 03:00    1.0817942550    2.1107085850  287.0797670000
99999999 06:00    1.0850368850    2.1017103250  287.0797670000
###    49.8287888889     8.7358333333    30.0000000000     0.0000000000     1     1     2
       2        3
DD FF TP
99999999 03:00    1.3031714750    2.7233556450  287.0797670000
99999999 06:00    1.3072397450    2.7123867650  287.0797670000
```

Comments

Line	Content and format
1st header	Model name, model version, test case, user name and model calculation are listed as strings within by apostrophes. No fixed format.
2nd header	First and last grid point index in x-direction, first and last grid point index in y-direction, first and last grid point index in z-direction. This information is not necessary for the test cases d1 and d2, but the line must be in the file even if the line is left empty. FORTRAN-format: (6(1X,I8))
1st data block row	The characters ### denote the begin of a new data block. This is followed by longitude and latitude [° decimal, western longitudes and southern latitudes are negative], height of the grid point above the ground [m], topography height below the grid point [m above sea level] and grid point index i, j, k in x-, y- and z-direction. For the test cases d1 and d2 the topography height and the grid point indices can be omitted. FORTRAN-format: (A3,4(1X,F16.10),3(1X,I8))
2nd data block row	Number of time steps and quantities within this data block. FOTRAN-format: (I8,1X,I8)
3rd data block row	identifiers of the quantities contained in this data block (see under key word *X_nclass_KK* in Section5.1.1). The following data block rows must contain the corresponding values of the quantities in the same order. FORTRAN-format: (n(A2,1X)) where n: number of identifiers
from 4th data block row onward	One data block row per time step (see 2nd data block row): Date [yyyymmdd] and time [hh:mm] of the model output and one value per quantity in the same order as stated in the 3rd data block row. If date and/or time are irrelevant, the fields have to be filled with “99999999“ resp. “99:99“. For quantities without any defined value ”-999.“ has to be stated for them. FORTRAN-format: (I8,1X,A5,n(1X,F15.10)) with n : number of quantities

The files with measured data provided by EVA (reference data sets for test cases d1 and d2) have apart from three differences a format analogous to the EVA-format:

- The 1st header contains only four fields: name of campaign, test case, user name and data of measuring data preparation.
- The 2nd header is empty or can be used for comments.
- The 1st data block row is terminated after the co-ordinates of the point of measurement.

A.2 Implemented VDI Criteria

The criteria implemented in the current EVA-version (Tables A.2.1 to A.2.8) correspond to the state of VID Guideline 3783 Sheet 7 as it was in November 2000, when it was still not finalised. If future changes in the programs are necessary due to differences between the final guideline and the one the current EVA is based on, these changes will be implemented into the program under a new version number.

Criteria Section 1 of the VDI-Guideline: Documentation
• Comprehensibility • Short Description of the Model • Long Description of the Model • Manual • Technical Reference
Criteria Section 2 of the VDI Guideline: Scientific Assessment
• u, v, w wind prognostic • Temperature prognostic • Specific humidity prognostic • Continuity equation or anelastic approximation • Buoyancy forces • Parameterisation of turbulence dependent on stability • Coriolis force • Fluxes are steady functions of location • Fluxes are steady functions of stratification • Surface fluxes are calculated directly or after MO-Theory • Symmetry of friction tensor • Explicit terrain height • Vegetation and buildings as roughness length • Three dimensional non-uniform grid • Surface following co-ordinates • Cloud microphysics • Ice phase • Subgridscale convection • Surface fluxes at least with „force-restore“ method • Surface humidity budget equation
Criteria Section 3 of the VDI-Guideline: Control of Model Calculations
• Grid structure • 2*DT waves • Standard deviations • Area average • Mass conservation • Validity range of model results • 2*DX, 2*DY waves • Results independent of grid • Plausibility

Table A.2.1: Implemented criteria for model properties

Quantity	***Symbol in EVA***	***Validation Limit R_0***	***Allowed Deviation D_0***
Wind direction	*DD*	*FF* > 1 m/s	0.1 °
Wind speed	*FF*	-	0.005 m/s
Potential temperature	*TP*	-	10^{-6} K

Table A.2.2: Implemented criteria for test case a

Quantity	***Symbol in EVA***	***Validation Limit R_0***	***Allowed Deviation D_0***
Wind direction	*DD*	*FF* > 1 m/s	1 °
Wind speed	*FF*	-	0.05 m/s
Potential temperature	*TP*	-	10^{-6} K

Table A.2.3: Implemented criteria for test case b1

Quantity	***Symbol in EVA***	***Validation Limit R_0***	***Allowed Deviation D_0***
Wind direction	*DD*	*FF* > 1 m/s	1 °
Wind speed	*FF*	-	0.05 m/s
Potential temperature	*TP*	-	0.01 K

Table A.2.4: Implemented criteria for test case b2

Quantity	***Symbol in EVA***	***Validation Limit R_0***	***Allowed Deviation D_0***
Wind direction	*DD*	*FF* > 1 m/s	40 °
Wind speed	*FF*	-	1.5 m/s
Pressure	*PP*	-	1.7 hPa
Relative humidity	*RH*	-	10 % absolute
Real temperature	*TT*	-	2 K
Vertical velocity	*WW*	-	0.1 m/s

Table A.2.5: Implemented criteria for test case d1

Quantity	***Symbol in EVA***	***Validation Limit R_0***	***Allowed Deviation D_0***
Wind direction	*DD*	*FF* > 1 m/s	40 °
Wind speed	*FF*	-	1.5 m/s
Pressure	*PP*	-	1.7 hPa
Relative humidity	*RH*	-	10 % absolute
Real temperature	*TT*	-	2 K
Vertical velocity	*WW*	-	0.1 m/s

Table A.2.6: Implemented criteria for test case d2

References

[1] VDI (2001): VDI 3783, Blatt 7: Prognostische mesoskalige nichthydrostatische Windfeldmodelle – Evaluierung für dynamisch und thermisch bedingte Strömungsfelder. *Kommission Reinhaltung der Luft im VDI und DIN, Beuth Verlag, Berlin*.

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[3] Bigalke, K., Schlünzen, K.H., Haenel, H.-D., Panskus H. (2001): Documentation of the model system METRAS^{+}. *Meteorologisches Institut, Universität Hamburg, METRAS Technical Rep. 12-E*.