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Description of the 3D LOTOS Model. Part I: Dynamics

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ABSTRACT
This report is part of the description of a tentative version of the three-dimensional regional air quality model LOTOS-HPCN. The starting-point of these models is the solution of the continuity equation that describes the change in concentration of a chemical species in the air as a result of transport, emissions, chemistry and some other processes. The physical domain of the model is part of a shell around the earth. In the vertical direction hybrid coordinates are used: the lower boundary is given by the orography of the earth and the upper boundary by a surface having equal pressure. For reasons of computational simplicity such an irregular physical domain is often transformed into a rectangular computational domain. The necessary transformation of the model equation is also described in this report.

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1. Description of the LOTOS model

LOTOS (LOng Term Ozone Simulation) is a three-dimensional Eulerian regional air quality model. The LOTOS model is driven by analyzed meteorological data and by an emission data base and is thought to be embedded in a larger model from which concentration values outside the LOTOS domain can be extracted. It is developed to simulate various chemical and physical processes in the troposphere / tropopause on a regional scale (≈ 1000 km).

The model is based on the equation for mass conservation of a chemical species c

$$c_t + \boldsymbol{\nabla} \cdot (\boldsymbol{u}c) = R + S, \tag{1.1}$$

where $\boldsymbol{u}$ is the given windfield, R describes the chemical reaction mechanism with the other species in the model and S denotes the source and sink terms. To account for turbulent fluctuations Reynolds (Favre) averaging of the flow variables – velocity u, density ρ, and mixing ratio χ ($c = \rho\chi$) – is used, which results in the model equation

$$c_t + \boldsymbol{\nabla} \cdot (\boldsymbol{u}c) = \boldsymbol{\nabla} \cdot (\rho K \boldsymbol{\nabla}\chi) + R + S \tag{1.2}$$

(see Appendix A). In (1.2) K is the eddy diffusivity tensor. The flow variables are now time-averaged quantities.

The domain of the model is part of a shell around the earth. The boundary surfaces are aligned with longitude and latitude coordinates and in the vertical direction defined by the 31-layer ECMWF hybrid coordinate system. So the domain is given by

$$\Omega = [\lambda_W, \lambda_E] \times [\phi_S, \phi_N] \times [z_{sfc}(\lambda, \phi), z_{top}(\lambda, \phi, t)], \tag{1.3}$$

where z_{sfc} is given by the orography and z_{top} is induced by z_{sfc} and by meteorological parameters.

It is assumed that the concentrations outside this domain are known, except of course at the surface of the earth. Here the boundary condition is determined by dry deposition

$$\mathbf{n} \cdot (\rho K \boldsymbol{\nabla} \chi) = v_d c, \tag{1.4}$$

where $\mathbf{n}$ is the unit vector normal to the surface and v_d is the deposition velocity.

1.1 The 31-layer ECMWF hybrid coordinate system

ECMWF[5] developed a hybrid coordinate system, which is terrain-following at the surface of the earth and has pressure levels at the top of the model. This coordinate system is induced by the surface pressure p_{sfc}, given at fixed time intervals Δt_{meteo}, and by the functions A and B given at the vertical layer boundaries (see Table 1). The pressure at the vertical grid points $\eta_{k+\frac{1}{2}}$ (cf. (1.11)) is given by

$$p_{k+\frac{1}{2}}(t_{meteo}) = A_{k+\frac{1}{2}} + B_{k+\frac{1}{2}} p_{sfc}(t_{meteo}), \quad k = 0, ..., N_\eta = 31, \tag{1.5}$$

where k is the vertical layer number.

The distance from the center of the earth to the vertical layer boundary is expressed by the function r. If a is the radius of the earth and z_{sfc} is defined by the orography then r is given at the discrete grid points by,

$$r(\eta_{N_\eta+\frac{1}{2}}, t) = a + z_{sfc}, \tag{1.6}$$

and for $k = 1, ..., N_\eta$ by

$$r(\eta_{k-\frac{1}{2}}, t_{meteo}) = a + z_{sfc} + z(\eta_{k-\frac{1}{2}}, t_{meteo}), \tag{1.7}$$

where

$$z(\eta_{k-\frac{1}{2}}, t_{meteo}) = \sum_{l=k}^{N_\eta} \int_{\eta_{l+\frac{1}{2}}}^{\eta_{l-\frac{1}{2}}} r_\eta d\eta. \tag{1.8}$$

To approximate the integral in the right-hand side the equation for hydrostatic pressure

$$dp = \rho g dz,$$

the ideal gas law, and the assumption that the mass of air does not depend on the percentage of water vapor are used. These assumptions give the following relation between the change of pressure and the vertical distance

$$dp = -\frac{p}{\gamma T} dz = -\frac{p}{\gamma T} r_\eta d\eta,$$

since the coordinate lines on which η varies coincide with the direction of the gravitational force. The integral in (1.8) can then be expressed by

$$\int_{\eta_{l+\frac{1}{2}}}^{\eta_{l-\frac{1}{2}}} r_\eta d\eta = -\gamma \int_{p_{l+\frac{1}{2}}}^{p_{l-\frac{1}{2}}} \frac{T}{p} dp \approx \gamma T_l(t_{meteo}) \log\left(\frac{p_{l+\frac{1}{2}}(t_{meteo})}{p_{l-\frac{1}{2}}(t_{meteo})}\right). \tag{1.9}$$

In Table 1 we give the vertical distances from the surface of the earth for $p_{sfc} = 1013$ and a given temperature profile.

1.1.1 Simplifying assumption The dependency of the function r on time t implies that r and the quantities dependent on r, like volume and cell faces of a grid cell, should be computed every time step. Even if we assume a linear relation between successive pressure values the r function can not be calculated using a linear relation. Therefore it seems justified to assume that the function r, and thus the physical grid changes only when new meteo data is read. A possible disadvantage is that the physical domain and consequently the physical volume of a grid cell changes discontinuously when new meteo data is read.

k	$A_{k+\frac{1}{2}}(Pa)$	$B_{k+\frac{1}{2}}$	$T(K)$	$p(hPa)$	$z(km)$
0	0.000000	0.0000000000	223.05	0.00	30.94270
1	2000.000000	0.0000000000	218.64	20.00	26.50887
2	4000.000000	0.0000000000	216.65	40.00	22.07504
3	6000.000000	0.0000000000	216.65	60.00	19.50507
4	8000.000000	0.0000000000	216.65	80.00	17.68165
5	9976.135361	0.0003908582	216.65	100.16	16.25734
6	11820.539617	0.0029197006	216.65	121.16	15.05055
7	13431.393926	0.0091941320	216.65	143.63	13.97249
8	14736.356909	0.0203191555	216.65	167.95	12.98103
9	15689.207458	0.0369748598	219.37	194.35	12.05563
10	16266.610500	0.0594876397	222.14	222.93	11.17511
11	16465.005734	0.0878949492	226.31	253.69	10.33505
12	16297.619332	0.1220035886	231.35	286.57	9.52819
13	15791.598604	0.1614415235	236.21	321.46	8.75054
14	14985.269630	0.2057032385	240.87	358.23	8.00204
15	13925.517858	0.2541886223	245.36	396.75	7.28236
16	12665.291662	0.3062353873	249.67	436.87	6.59087
17	11261.228878	0.3611450218	253.80	478.45	5.92675
18	9771.406290	0.4182022749	257.77	521.35	5.28914
19	8253.212096	0.4766881754	261.58	565.42	4.67725
20	6761.341326	0.5358865832	265.23	610.47	4.09058
21	5345.914240	0.5950842740	268.70	656.28	3.52908
22	4050.717678	0.6535645569	272.01	702.57	2.99330
23	2911.569385	0.7105944258	275.12	748.95	2.48458
24	1954.805296	0.7654052430	278.02	794.90	2.00527
25	1195.889791	0.8171669567	280.67	839.75	1.55887
26	638.148911	0.8649558510	283.04	882.58	1.15037
27	271.626545	0.9077158297	285.06	922.23	0.78647
28	72.063577	0.9442132326	286.65	957.21	0.47604
29	0.000000	0.9729851852	287.73	985.63	0.23063
30	0.000000	0.9922814815	288.15	1005.18	0.06532
31	0.000000	1.0000000000	288.15	1013.00	0.00000

Table 1: Constants A and B defining the ECMWF hybrid coordinates. The last two columns give the pressure and the distance from the surface of the earth for $p_{sfc} = 1013$ and the given temperature profile.

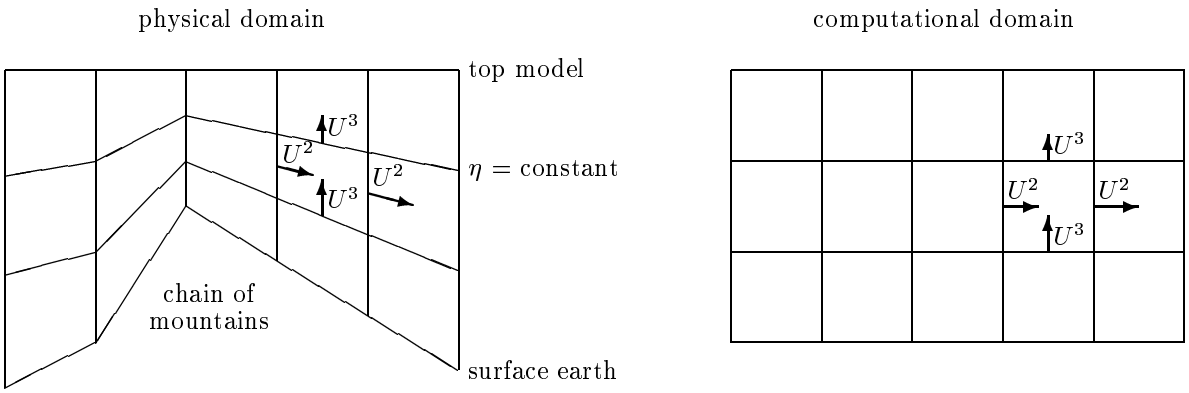

Figure 1: Slice $\lambda = constant$ through physical and computational domain with contravariant velocity components (courtesy: Edwin Spee).

1.2 Derivation of the LOTOS model for the computational domain

The physical domain on which equation (1.2) has to be solved is thus defined by space (and time) dependent input variables, viz., the orography of the earth and the surface pressure. For such an arbitrary physical domain it is often worthwhile to solve the problem in a boundary-conforming curvilinear coordinate system, i.e., to transform the *physical domain*, regardless of its shape in physical space, to a fixed rectangular *computational domain* such that a *physical boundary segment* coincides with a *coordinate line in computational space* (see Fig. 1). Of course the model equations must be transformed to the curvilinear coordinate system, but the resulting equations are of the same type, although more complicated, as the original ones. On the fixed rectangular grid the transformed problem can then be discretized and solved using standard numerical techniques.

1.2.1 The computational grid and the coordinate transformation We want to transform the *physical* domain

$$\Omega = [\lambda_W, \lambda_E] \times [\phi_S, \phi_N] \times [z_{sfc}(\lambda, \phi), z_{top}(\lambda, \phi)], \tag{1.10}$$

to a *computational domain* defined by the *uniform* longitude-latitude-hybrid *computational* grid where the cell centers are given by

$$\Gamma = \{(\lambda_i, \phi_j, \eta_k) |\ i = 1, ..., N_\lambda,\ j = 1, ..., N_\phi,\ k = 1, ..., N_\eta\}, \tag{1.11}$$

with $\Delta\lambda = (\lambda_E - \lambda_W)/N_\lambda$, $\lambda_1 = \lambda_W + \Delta\lambda/2$, $\Delta\phi = (\phi_N - \phi_S)/N_\phi$, $\phi_1 = \phi_S + \Delta\phi/2$, and $\Delta\eta = 1.0/N_\eta$, $\eta_1 = 1.0 - \Delta\eta/2$.

The transformation between the Cartesian coordinate system (X, Y, Z) defined on Ω and the curvilinear coordinate system defined by Γ is given by

$$\begin{aligned} X(\lambda, \phi, \eta) &= r(\lambda, \phi, \eta)\cos\phi\cos\lambda, \\ Y(\lambda, \phi, \eta) &= r(\lambda, \phi, \eta)\cos\phi\sin\lambda, \\ Z(\lambda, \phi, \eta) &= r(\lambda, \phi, \eta)\sin\phi. \end{aligned} \tag{1.12}$$

Note that the longitude-latitude-hybrid coordinate system is *not* orthogonal.

Since the function r is given only at discrete points in space by equations (1.7) and (1.8) we have to define a continuation of r to compute, e.g., the volume and cell faces of a grid cell. We use the simplest possible *continuous* continuation of r on a boundary surface in the vertical direction, viz., trilinear splines

$$r(\lambda, \phi, \eta) = \sum_{i=0}^{N_\lambda} \sum_{j=0}^{N_\phi} \sum_{k=0}^{N_\eta} r(\lambda_{i+\frac{1}{2}}, \phi_{j+\frac{1}{2}}, \eta_{k+\frac{1}{2}}) \psi_{i+\frac{1}{2}}(\lambda) \psi_{j+\frac{1}{2}}(\phi) \psi_{k+\frac{1}{2}}(\eta), \tag{1.13}$$

where

$$\psi_{i+\frac{1}{2}}(\lambda) = \begin{cases} 0 & \lambda \notin (\lambda_{i-\frac{1}{2}}, \lambda_{i+\frac{3}{2}}) \\ \frac{\lambda - \lambda_{i-\frac{1}{2}}}{\Delta\lambda} & \lambda \in (\lambda_{i-\frac{1}{2}}, \lambda_{i+\frac{1}{2}}) \\ \frac{\lambda_{i+\frac{3}{2}} - \lambda}{\Delta\lambda} & \lambda \in (\lambda_{i+\frac{1}{2}}, \lambda_{i+\frac{3}{2}}) \end{cases} \tag{1.14}$$

and $\psi_{j+\frac{1}{2}}(\phi)$ and $\psi_{k+\frac{1}{2}}(\eta)$ are defined analogously. So we assume that p_{sfc} is given in the surface grid points and that the temperature is given between two vertical grid points.

1.2.2 The LOTOS model In Appendix B we describe how to transform an equation defined in a Cartesian coordinate system to a general curvilinear coordinate system. Here we give only the resulting formulas for the LOTOS model.

The transformation is characterized by the so-called *metric tensors* that are associated with the base vectors of the curvilinear coordinate system defined by (1.11). The *covariant* metric tensor (g_{ij}) equals

$$\begin{pmatrix} r^2\cos^2\phi + {r_\lambda}^2 & r_\lambda r_\phi & r_\lambda r_\eta \\ r_\lambda r_\phi & r^2 + {r_\phi}^2 & r_\phi r_\eta \\ r_\lambda r_\eta & r_\phi r_\eta & {r_\eta}^2 \end{pmatrix}. \tag{1.15}$$

A frequently used quantity, connected with an increment of volume, is the *Jacobian* of the transformation, which is given by

$$\sqrt{g} \equiv \det(g_{ij}) = r^2 r_\eta \cos\phi. \tag{1.16}$$

Finally, the *contravariant* metric tensor (g^{ij}) is

$$\begin{pmatrix} \frac{1}{r^2\cos^2\phi} & 0 & -\frac{r_\lambda}{r^2 r_\eta \cos^2\phi} \\ 0 & \frac{1}{r^2} & -\frac{r_\phi}{r^2 r_\eta} \\ -\frac{r_\lambda}{r^2 r_\eta \cos^2\phi} & -\frac{r_\phi}{r^2 r_\eta} & \frac{r^2\cos^2\phi + {r_\phi}^2\cos^2\phi + {r_\lambda}^2}{r^2 {r_\eta}^2 \cos^2\phi} \end{pmatrix}. \tag{1.17}$$

The transformation of the model equation (1.2) to the new coordinate system results in (cf. equation (B.35b))

$$(\sqrt{g}c)_t + \sum_{i=1}^{3}(U^i\sqrt{g}c)_{\xi^i} = \sum_{i=1}^{3}\sum_{j=1}^{3}[\sqrt{g}\rho K^{ij}\chi_{\xi^j}]_{\xi^i} + \sqrt{g}R + \sqrt{g}S,$$

where K^{ij} are the contravariant components of the eddy diffusivity tensor.

If we assume that K^{ij} has only diagonal elements we arrive at the governing model equation in the longitude-latitude-hybrid coordinate system for each chemical species c in the LOTOS model

$$(\sqrt{g}c)_t + \sum_{i=1}^{3}(U^i\sqrt{g}c)_{\xi^i} = \sum_{i=1}^{3}[\sqrt{g}\rho K^{ii}\chi_{\xi^i}]_{\xi^i} + \sqrt{g}R + \sqrt{g}S, \tag{1.18}$$

where ρ denotes the density, χ is the mixing ratio, K^{ii} are contravariant eddy diffusion coefficients, R describes the chemical reaction mechanism between the species in the model and S denotes source and sink terms. The quantity U^i is the contravariant velocity component in the ξ^i-direction, where $\xi^1 = \lambda$, $\xi^2 = \phi$, and $\xi^3 = \eta$. The upper indices 1, 2, 3 and i are not exponents but superscripts indicating a specific coordinate. Note that the conservative form is used.

The computational domain is defined by the *uniform* longitude-latitude-hybrid grid (1.11).

Equations (1.18) will be discretized and solved in all grid points of Γ except for the boundary surface $\eta = 0$ and the top layers $k = 1, ..., k_0 >= 3$. It is assumed that all values, needed in the discretization,

outside the computational domain are available, e.g., generated by an enveloping model. For $\eta = 0$ the boundary condition is

$$\frac{1}{\sqrt{g^{33}}}\rho K^{33}\chi_\eta = v_d c, \tag{1.19}$$

where v_d is the deposition velocity which will be specified elsewhere.

NB. In the above two assumptions are made that differ from the ones in the 'old' 2D 3-layer LOTOS model (see, e.g., [2],[6]):

1. In the new LOTOS model it is *not* assumed that the windfield is divergence-free.
2. It is assumed that the *contravariant* diffusion tensor is diagonal, whereas in the 2D LOTOS model the diffusion tensor is assumed to be diagonal in the spherical coordinate system.

Analogous with the old LOTOS model the contravariant horizontal eddy diffusivities K^{11} and K^{22} are parameterized in the model by

$$\begin{aligned} K^{ll} = g^{ll}\varepsilon \quad & \left([(\sqrt{g_{22}}U^2)_\lambda/\sqrt{g_{11}} + (\sqrt{g_{11}}U^1)_\phi/\sqrt{g_{22}}]^2 + \right. \\ & \left. [(\sqrt{g_{11}}U^1)_\lambda/\sqrt{g_{11}} - (\sqrt{g_{22}}U^2)_\phi/\sqrt{g_{22}}]^2\right)^{\frac{1}{2}}, \end{aligned} \tag{1.20}$$

where $\varepsilon = 9000\, m^2$ is an empirical constant based on scale considerations, and g^{ll} and g_{ii} are defined in (1.17) and (1.15), respectively.

The vertical diffusion is modeled by the parameterization of Louis[4] which was also used in the ECMWF [5]), the ECHAM3 [1], and the TM2 [3] models.

The vertical diffusion coefficient K_{33} is given by

$$K_{33} = g^{33} l_h^2 \left([(\sqrt{g_{11}}U^1)_\eta/\sqrt{g_{33}}]^2 + [(\sqrt{g_{22}}U^2)_\eta/\sqrt{g_{33}}]^2\right)^{\frac{1}{2}} f(R_b), \tag{1.21}$$

with different functions f for stable ($R_b > 0$) or unstable ($R_b < 0$) conditions. The mixing length l_h is given by

$$l_h = \frac{\kappa z}{1 + \kappa z/\lambda_h}, \tag{1.22}$$

where z is the height above the ground, κ is the von Karman constant (=0.4) and the asymptotic mixing length $\lambda_h = 438.18m$. Dry air is assumed in the computation of the bulk Richardson number

$$R_b(z) = \frac{g\Delta z(C_{pd}\Delta T + g\Delta z)}{C_{pd}T|\Delta \boldsymbol{U}|^2}. \tag{1.23}$$

Here, ΔT is the temperature difference and $\Delta \boldsymbol{U}$ the vertical wind shear over the vertical layer around z with height Δz ($|\Delta \boldsymbol{U}_k|^2 = [U^1_{k+\frac{1}{2}} - U^1_{k-\frac{1}{2}}]^2 + [U^2_{k+\frac{1}{2}} - U^2_{k-\frac{1}{2}}]^2 + [U^3_{k+\frac{1}{2}} - U^3_{k-\frac{1}{2}}]^2$). The specific heat of dry air at constant pressure $C_{pd} = 1005.46 J\, kg^{-1}\, K^{-1}$ and the acceleration of gravity $g = 9.80665 m\, s^{-2}$.

The stability function $f(R_b)$ is computed according to the sign of R_b. In the stable case ($R_b > 0$) f is given by

$$f(R_b) = \frac{1}{1 + 3bR_b\sqrt{1 + dR_b}}, \tag{1.24}$$

and in the unstable case ($R_b <= 0$)

$$f(R_b) = 1 - \frac{3bR_b}{1 + G(R_b)}, \tag{1.25}$$

where

$$G(R_b) = 3be l_h^2 \left[\frac{-R_b}{z}\left(\frac{1}{\Delta z}\left[(1 + \frac{\Delta z}{z})^{\frac{1}{3}} - 1\right]\right)^3\right]^{\frac{1}{2}}, \tag{1.26}$$

with $b = d = e = 5$ and Δz is the distance between adjacent model layers.

A. Reynolds decomposition

The equation for mass conservation of a chemical species c is given by

$$c_t + \boldsymbol{\nabla} \cdot (\boldsymbol{u}c) = S, \tag{A.1}$$

where $\boldsymbol{u}$ is a given windfield and S denotes source and sink terms.

To account for turbulent fluctuations in a flow one often uses the so-called Reynolds decomposition of the flow variables, i.e., a flow variable is decomposed into a mean and a fluctuating component

$$q = \overline{q} + q',$$

where q' is the fluctuation in time of the quantity and $\overline{q}$ is the time-averaged mean of q given by

$$\overline{q} = \frac{1}{\Delta t} \int_t^{t+\Delta t} q d\tau.$$

It is clear that $\overline{q'} = 0$. Note however, that the time average of nonlinear combinations like $\overline{q'q'}$ is not zero.

The quantities of interest in the mass-conservation equation are the windfield u and the species c, or rather the density ρ and the mixing ratio χ ($c = \rho\chi$). If we apply the Reynolds decomposition for these three variables we would end up with triple correlations involving the density fluctuations. To avoid this the so-called Favre-average or 'density-weighted' approach is used. In this approach the velocity and the mixing ratio are decomposed into a mean and a fluctuating component

$$q = \tilde{q} + q'',$$

with the requirement that the time average $\overline{\rho q''} = 0$, which implies that

$$\tilde{q} = \frac{\overline{\rho q}}{\rho}.$$

The time-average of the product $\rho u \chi$ then contains only one term caused by the fluctuations

$$\overline{\rho u \chi} = \overline{\rho(\tilde{u} + u'')(\tilde{\chi} + \chi'')} = \overline{\rho}\tilde{u}\tilde{\chi} + \overline{\rho u'' \chi''}.$$

Note, that for constant density, i.e., $\rho' = 0$, the two approaches are the same.

Substituting the decomposed variables in the continuity equation (A.1) gives

$$(\rho(\tilde{\chi} + \chi''))_t + \boldsymbol{\nabla} \cdot (\rho(\tilde{u} + u'')(\tilde{\chi} + \chi'')) = S(\rho(\tilde{\chi} + \chi'')).$$

If we take the time average of this equation and neglect higher order terms in the source and sink terms we get

$$(\overline{\rho}\tilde{\chi})_t + \boldsymbol{\nabla} \cdot (\overline{\rho}\tilde{u}\tilde{\chi}) + \boldsymbol{\nabla} \cdot (\overline{\rho u'' \chi''}) = S(\overline{\rho}\tilde{\chi}). \tag{A.2}$$

Thus the time average of the product of the fluctuating variables represents the turbulent flux and the divergence of this flux affects the mean concentration.

In general, the divergence of the turbulent fluxes is parameterized in the form of gradient diffusion

$$\boldsymbol{\nabla} \cdot (\overline{\rho u'' \chi''}) \approx -\boldsymbol{\nabla} \cdot (\overline{\rho K} \boldsymbol{\nabla} \overline{\chi}), \tag{A.3}$$

where K is the eddy diffusivity tensor to be specified. For convenience, the bars over the variables are often omitted, but it should be kept in mind that the variables denote time-averaged quantities.

B. Transformation of a convection-diffusion-reaction equation

The generic form of a convection-diffusion-reaction equation is

$$c_t + \boldsymbol{\nabla} \cdot (\boldsymbol{u}c) = \boldsymbol{\nabla} \cdot (K \boldsymbol{\nabla} c) + R. \tag{B.1}$$

The boundary conditions belonging to system (B.1) are of the form

$$\alpha c + \beta \mathbf{n} \cdot (K \boldsymbol{\nabla} c) = \gamma. \tag{B.2}$$

If the physical domain is defined by time and space dependent input variables it is often better to solve the problem in a boundary-conforming curvilinear coordinate system, i.e., to transform the *physical domain*, regardless of its shape and movement in physical space, to a fixed rectangular *computational domain* such that a *physical boundary segment* coincides with a *coordinate line in computational space*. Of course the equations (B.1-B.2) must be transformed to the curvilinear coordinate system too.

B.1 Coordinate transformation relations

In this section we describe the transformation relations needed to transform equations (B.1-B.2) from physical Cartesian coordinates (x_1, x_2, x_3, t) to a general curvilinear coordinate system (ξ^1, ξ^2, ξ^3, t). Note that the numbers 1, 2, 3 are not exponents but superscripts indicating a specific coordinate. This is the customary notation for general (non-rectangular) coordinate systems. The contents of this section is borrowed from the book Numerical Grid Generation by Thompson, Warsi, and Mastin[7].

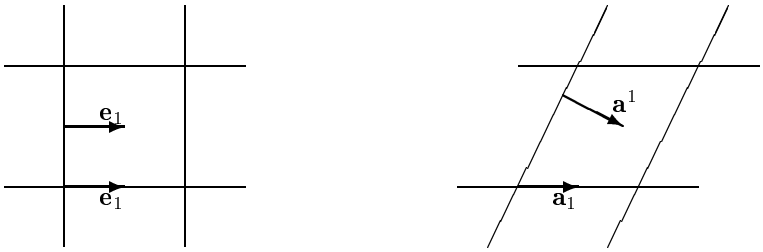

Figure 2: Rectangular (left) and oblique (right) coordinate system in 2D with (unique) unit vector $\mathbf{e}_1$, and covariant and contravariant base vectors, $\mathbf{a}_1$ and $\mathbf{a}^1$, respectively. For orthogonal and general curvilinear coordinate systems the unit vector and the co- and contravariant base vectors are local, i.e., they can be different for each coordinate point.

It is assumed that there exists a 1-1 mapping of the physical region onto the transformed region, that coordinate lines of the same family do not cross, and that coordinate lines of different families do not cross more than once. The curvilinear coordinate lines are space curves formed by the intersection of surfaces on which one coordinate is constant. So along a coordinate line one coordinate varies while the other two are constant. Base vectors of the coordinate system are the tangents to the coordinate line (the *covariant* base vectors) and the normals to the coordinate surface (the *contravariant* base vectors). These two type of base vectors are parallel if and only if the coordinate system is orthogonal (see Fig. 2).

In the following a variable with a coordinate as subscript means the derivative of the variable with respect to that coordinate.

The *covariant* base vectors are given by

$$\mathbf{a}_i \equiv \boldsymbol{r}_{\xi^i}, \quad i = 1, 2, 3, \tag{B.3}$$

where the *subscript* i indicates the base vector corresponding to the ξ^i coordinate, i.e., the tangent of the coordinate line along which only ξ^i varies.

The *contravariant* base vectors are given by

$$\mathbf{a}^i \equiv \boldsymbol{\nabla}\xi^i, \quad i = 1,2,3, \tag{B.4}$$

where the *superscript* i indicates the base vector corresponding to the coordinate surface on which ξ^i is constant.

Associated with the base vectors are symmetric metric tensors with as components the dot products of the respective base vectors. Thus we have the *covariant* metric tensor with components:

$$g_{ij} = \mathbf{a}_i \cdot \mathbf{a}_j, \quad i,j = 1,2,3, \tag{B.5}$$

and the *contravariant* metric tensor with components:

$$g^{ij} = \mathbf{a}^i \cdot \mathbf{a}^j, \quad i,j = 1,2,3. \tag{B.6}$$

The contravariant base vectors can be written in terms of the covariant base vectors as

$$\mathbf{a}^i = \frac{1}{\sqrt{g}}\mathbf{a}_j \times \mathbf{a}_k, \quad i = 1,2,3, \ (i,j,k) \text{ cyclic}, \tag{B.7}$$

where $\sqrt{g}$, called the *Jacobian* of the transformation, is given by

$$\sqrt{g} \equiv \sqrt{\det|g_{ij}|} = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3). \tag{B.8}$$

A useful relation between covariant and contravariant metrics is

$$\mathbf{a}_i \cdot \mathbf{a}^j = \delta_i^j. \tag{B.9}$$

This relation implies that any vector $\boldsymbol{v}$ can be expressed in terms of either set of base vectors as

$$\boldsymbol{v} = \sum_{i=1}^{3}(\mathbf{a}_i \cdot \boldsymbol{v})\mathbf{a}^i \tag{B.10}$$

and

$$\boldsymbol{v} = \sum_{i=1}^{3}(\mathbf{a}^i \cdot \boldsymbol{v})\mathbf{a}_i \tag{B.11}$$

$v_i = \mathbf{a}_i \cdot \boldsymbol{v}$ and $v^i = \mathbf{a}^i \cdot \boldsymbol{v}$ are called the covariant and contravariant components of the vector $\boldsymbol{v}$.

Some other relations:

$$\det|g^{ij}| = \frac{1}{\det|g_{ij}|} = \frac{1}{g}, \tag{B.12}$$

$$\sum_{i=1}^{3}(\mathbf{a}_j \times \mathbf{a}_k)_{\xi^i} = \sum_{i=1}^{3}(\sqrt{g}\mathbf{a}^i)_{\xi^i} = 0. \tag{B.13}$$

The differential elements of arc length, surface and volume can be generated directly from the covariant base vectors. The general differential increment of a position vector is given by

$$d\boldsymbol{r} = \sum_{i=1}^{3}\boldsymbol{r}_{\xi^i}d\xi^i = \sum_{i=1}^{3}\mathbf{a}_i d\xi^i. \tag{B.14}$$

An increment of arc length along a general space curve is then given by

$$(ds)^2 = |d\boldsymbol{r}|^2 = \sum_{i=1}^{3}\sum_{j=1}^{3}\mathbf{a}_i \cdot \mathbf{a}_j d\xi^i d\xi^j = \sum_{i=1}^{3}\sum_{j=1}^{3}g_{ij}d\xi^i d\xi^j \tag{B.15}$$

An increment of arc length on a coordinate line along which ξ^i varies is given by

$$ds_i = |\boldsymbol{r}_{\xi^i}|d\xi^i = |\mathbf{a}_i|d\xi^i = \sqrt{g_{ii}}d\xi^i \tag{B.16}$$

An increment of area on a coordinate surface of constant ξ^i is given by

$$dS_i = |\boldsymbol{r}_{\xi^j} \times \boldsymbol{r}_{\xi^k}|d\xi^j d\xi^k = |\mathbf{a}_j \times \mathbf{a}_k|d\xi^j d\xi^k = \sqrt{g_{jj}g_{kk} - g_{jk}^2}d\xi^j d\xi^k. \tag{B.17}$$

An increment of volume is given by

$$dV = \boldsymbol{r}_{\xi^i} \cdot (\boldsymbol{r}_{\xi^j} \times \boldsymbol{r}_{\xi^k})d\xi^i d\xi^j d\xi^k = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)d\xi^1 d\xi^2 d\xi^3 = \sqrt{g}d\xi^1 d\xi^2 d\xi^3. \tag{B.18}$$

Expressions for the derivative operators, such as gradient, divergence, curl, Laplacian, etc., are obtained by applying the Divergence Theorem of Gauß to a differential volume increment bounded by coordinate surfaces. We give here only the expressions needed for the transformation of equations (B.1-B.2) in conservative form. The expression for the gradient will be derived, the other ones can be obtained analogously.

A corollary of the divergence theorem

$$\iiint_V \boldsymbol{\nabla} \cdot \boldsymbol{v} dV = \iint_S \boldsymbol{v} \cdot \mathbf{n} dS \tag{B.19}$$

is

$$\iiint_V \boldsymbol{\nabla} c dV = \iint_S c\,\mathbf{n} dS, \tag{B.20}$$

where the volume V is enclosed by the surface S and $\mathbf{n}$ is the outward-directed unit normal to S. Consider a differential element of volume, δV, bounded by six cell faces lying on coordinate surfaces, then the following equation holds for the product of $\mathbf{n}$ and a differential surface element (cf. (B.17))

$$\mathbf{n}dS_i = \pm \mathbf{a}_j \times \mathbf{a}_k d\xi^j d\xi^k. \tag{B.21}$$

With this equation and equation(B.18) we get for (B.20)

$$\iiint_{\delta V} \boldsymbol{\nabla} c \sqrt{g} d\xi^1 d\xi^2 d\xi^3 = \sum_{i=1}^{3} \left(\iint_{\delta S_i^+} c(\mathbf{a}_j \times \mathbf{a}_k)d\xi^j d\xi^k - \iint_{\delta S_i^-} c(\mathbf{a}_j \times \mathbf{a}_k)d\xi^j d\xi^k \right). \tag{B.22}$$

Taking the limit for $\delta V \to 0$ gives the expression for the gradient of c.
Gradient:

$$\boldsymbol{\nabla} c = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\sqrt{g}\mathbf{a}^i c)_{\xi^i}. \tag{B.23}$$

Divergence:

$$\boldsymbol{\nabla} \cdot \boldsymbol{v} = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} (\sqrt{g}\mathbf{a}^i \cdot \boldsymbol{v})_{\xi^i}. \tag{B.24}$$

Laplacian:

$$\boldsymbol{\nabla}^2 c = \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} c) = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{j=1}^{3} [\mathbf{a}^i \cdot (\sqrt{g}\mathbf{a}^j c)_{\xi^j}]_{\xi^i}. \tag{B.25}$$

Derivatives:

$$c_{x_j} = (\boldsymbol{\nabla} c)_j = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} [\sqrt{g}(\mathbf{a}^i)_j c]_{\xi^i} \tag{B.26}$$

$$c_{x_j x_k} = [\boldsymbol{\nabla}(c_{x_j})]_k = \frac{1}{\sqrt{g}} \sum_{i=1}^{3} \sum_{l=1}^{3} \{(\mathbf{a}^i)_k [\sqrt{g}(\mathbf{a}^l)_j c]_{\xi^l}\}_{\xi^i}. \tag{B.27}$$

For the boundary conditions we need expressions for the derivatives normal and tangential to coordinate surfaces. The tangential derivative on a coordinate line along which ξ^i varies is given by (since $(\boldsymbol{u} \times \boldsymbol{v}) \times \boldsymbol{w} = \boldsymbol{v}(\boldsymbol{u} \cdot \boldsymbol{w}) - \boldsymbol{u}(\boldsymbol{v} \cdot \boldsymbol{w})$)

$$(c)^i_\tau \equiv \frac{\mathbf{a}_i}{|\mathbf{a}_i|} \cdot \boldsymbol{\nabla} c = \frac{c_{\xi^i}}{\sqrt{g_{ii}}}, \qquad (i,j,k) \text{ cyclic.} \tag{B.28}$$

The normal derivative to a coordinate surface on which ξ^i is constant is given by

$$(c)^i_n \equiv \frac{\mathbf{a}^i}{|\mathbf{a}^i|} \cdot \boldsymbol{\nabla} c = \frac{1}{\sqrt{g^{ii}}} \sum_{j=1}^{3} g^{ij} c_{\xi^j}. \tag{B.29}$$

The derivative normal to the coordinate line along which ξ^i varies and tangent to the coordinate surface on which ξ^i is constant is given by

$$(c)^i_T \equiv \frac{\mathbf{a}^i \times \mathbf{a}_i}{|\mathbf{a}^i \times \mathbf{a}_i|} \cdot \boldsymbol{\nabla} c = \frac{g_{ij} c_{\xi^k} - g_{ik} c_{\xi^j}}{\sqrt{g_{ii}(g_{jj} g_{kk} - g_{jk}^2) - g}}. \tag{B.30}$$

Finally, we need the first derivative in time:

$$(c_t)^{\boldsymbol{x}} = (c_t)^{\boldsymbol{\xi}} - \boldsymbol{\nabla} c \cdot (\boldsymbol{x}_t)^{\boldsymbol{\xi}}, \tag{B.31}$$

where the superscripts indicate the variable being held constant in the partial differentiation. So the time derivative on the right-hand side is at a fixed point in the transformed or computational space, i.e., at a given grid point. The time derivative on the left-hand side is at a fixed point in physical space, i.e., the time derivative that appears in the physical equations of motion. The grid point speed is given by

$$\dot{\boldsymbol{x}} \equiv (\boldsymbol{x}_t)^{\boldsymbol{\xi}}. \tag{B.32}$$

B.2 The convection-diffusion-reaction equation in a curvilinear coordinate system
With all these relations we can now transform the generic form of the convection-diffusion-reaction equation (B.1)

$$c_t + \boldsymbol{\nabla} \cdot (\boldsymbol{u} c) = \boldsymbol{\nabla} \cdot (K \boldsymbol{\nabla} c) + R,$$

or alternatively written

$$c_t + \sum_{i=1}^{3} (u_i c)_{x_i} = \sum_{i=1}^{3} [\mathbf{e}_i \cdot K \sum_{j=1}^{3} (\mathbf{e}_j c_{x_j})]_{x_i} + R, \tag{B.33}$$

where $\mathbf{e}_1 \equiv \mathbf{i}$, $\mathbf{e}_2 \equiv \mathbf{j}$, and $\mathbf{e}_3 \equiv \mathbf{k}$. The diffusion parameter K can be a scalar or a tensor. In the curvilinear coordinate system the conservative form of the convection-diffusion-reaction equation is given by

$$(\sqrt{g} c)_t + \sum_{i=1}^{3} (U^i \sqrt{g} c)_{\xi^i} = \sum_{i=1}^{3} [\mathbf{a}^i \cdot K \sum_{j=1}^{3} (\sqrt{g} \mathbf{a}^j c)_{\xi^j}]_{\xi^i} + \sqrt{g} R. \tag{B.34}$$

Expanding the inner derivative in the diffusion term gives an expression which is still conservative with respect to the ξ^i-derivatives and which is given for a scalar K by

$$(\sqrt{g}c)_t + \sum_{i=1}^{3}(U^i\sqrt{g}c)_{\xi^i} = \sum_{i=1}^{3}\sum_{j=1}^{3}[K\sqrt{g}g^{ij}c_{\xi^j}]_{\xi^i} + \sqrt{g}R. \tag{B.35a}$$

For a tensor K represented by its contravariant components

$$K = K^{lm}\mathbf{a}_l\mathbf{a}_m = \sum_{l=1}^{3}\sum_{m=1}^{3} K^{lm}\mathbf{a}_l(\mathbf{a}_m)^T$$

the diffusion term reads

$$\begin{aligned}
\sqrt{g}\boldsymbol{\nabla}\cdot(K\boldsymbol{\nabla}c) &= \sum_{i,j}[\sqrt{g}\mathbf{a}^i\cdot\sum_{l,m}K^{lm}\mathbf{a}_l(\mathbf{a}_m)^T\mathbf{a}^j c_{\xi^j}]_{\xi^i} \\
&= \sum_{i,j}[\sqrt{g}\mathbf{a}^i\cdot\sum_{l,m}K^{lm}\mathbf{a}_l(\mathbf{a}_m\cdot\mathbf{a}^j)c_{\xi^j}]_{\xi^i} \\
&= \sum_{i,j}[\sqrt{g}\mathbf{a}^i\cdot\sum_{l}K^{lj}\mathbf{a}_l c_{\xi^j}]_{\xi^i} = \sum_{i,j}[\sqrt{g}K^{ij}c_{\xi^j}]_{\xi^i},
\end{aligned}$$

so that equation (B.34) for a contravariant tensor K^{ij} is given by

$$(\sqrt{g}c)_t + \sum_{i=1}^{3}(U^i\sqrt{g}c)_{\xi^i} = \sum_{i=1}^{3}\sum_{j=1}^{3}[\sqrt{g}K^{ij}c_{\xi^j}]_{\xi^i} + \sqrt{g}R. \tag{B.35b}$$

If K^{ij} has only diagonal elements this simplifies into

$$(\sqrt{g}c)_t + \sum_{i=1}^{3}(U^i\sqrt{g}c)_{\xi^i} = \sum_{i=1}^{3}[\sqrt{g}K^{ii}c_{\xi^i}]_{\xi^i} + \sqrt{g}R. \tag{B.35c}$$

Equation (B.35) shows that after transformation the product $(\sqrt{g}c)$ is conserved rather than the function c itself. The time derivative in (B.35) is understood to be at a fixed point in computational space. The quantity

$$U^i = \mathbf{a}^i\cdot(\boldsymbol{u} - \dot{\boldsymbol{x}}) \tag{B.36}$$

is the contravariant velocity component in the ξ^i-direction, relative to the moving grid. Note that the equation for divergence freedom of the windfield $\boldsymbol{u}$ is transformed into

$$\sum_{i=1}^{3}\mathbf{a}^i\cdot(\boldsymbol{u}_{\xi^i}) = 0. \tag{B.37}$$

Finally, the boundary condition (B.2)

$$\alpha c + \beta\mathbf{n}\cdot(K\boldsymbol{\nabla}c) = \gamma.$$

is transformed into

$$\alpha c + \beta\frac{1}{\sqrt{g^{ii}}}\sum_{j=1}^{3}K^{ij}c_{\xi^j} = \gamma \tag{B.38}$$

for a boundary on which ξ^i is constant (for scalar K: $K^{ij} = K\,g^{ij}$).

B.3 Discrete representation

If the transformed equations are solved in conservative form it is important that the discretization should be such that numerically the identities (B.13) and

$$(\sqrt{g})_t = \sqrt{g} \sum_{i=1}^{3} \mathbf{a}^i \cdot (\dot{\boldsymbol{x}})_{\xi^i}$$

hold. Otherwise spurious oscillations will be introduced, since the numerical derivatives of constant physical quantities are nonzero.

It is possible that a numerical evaluation of the metric coefficients is better than the 'exact' evaluation. Spurious oscillations can be partially corrected by subtracting off the product of the metric identities with either a uniform solution or the local solution. A code should be checked with constant c to detect this kind of metric errors.

C. List of symbols

symbol	meaning	(defining) equation	units
λ_W, λ_E	zonal domain boundaries	(1.3) (1.11)	$radian$
ϕ_S, ϕ_N	meridional domain boundaries	(1.3) (1.11)	$radian$
$z_{sfc}(\lambda,\phi)$, $z_{top}(\lambda,\phi,t)$	vertical boundaries physical domain	(1.3)	m
λ	zonal variable	(1.11)	$radian$
ϕ	meridional variable	(1.11)	$radian$
z	vertical variable physical domain	(1.8)	m
η	vertical variable computational grid	(1.11)	
$r(\lambda,\phi,\eta)$	distance from center of earth	(1.7)	m
$i = 1,...,N_\lambda$	zonal index	(1.11)	
$j = 1,...,N_\phi$	meridional index	(1.11)	
$k = k_0,...,N_\eta$	vertical index	(1.11)	
t	time		s
$\sqrt{g}$	Jacobian of domain transformation	(1.16)	
(g_{ij})	covariant metric tensor transformation	(1.15)	
(g^{ij})	contravariant metric tensor transformation	(1.17)	
$\rho(\lambda,\phi,\eta,t)$	density of air	(1.18)	$kg\,m^{-3}$
$c(\lambda,\phi,\eta,t)$	concentration of chemical species	(1.18)	$kg\,m^{-3}$
$\chi(\lambda,\phi,\eta,t)$	mixing ratio (c/ρ)	(1.18)	
$U^i(\lambda,\phi,\eta,t)$	contravariant component of wind velocity	(1.18)	$m\,s^{-1}$
$K^{ii}(\lambda,\phi,\eta,t)$	contravariant eddy diffusion coefficients	(1.18)	$m^2\,s^{-1}$
$S(\lambda,\phi,\eta,t)$	chemical sources and sinks	(1.18)	$kg\,m^{-3}\,s^{-1}$
v_d	deposition velocity	(1.19)	$m\,s^{-1}$
l_h	mixing length for heat (scalars)	(1.22)	m
λ_h	asymptotic mixing length for heat (scalars)	(1.22)	m
$p_{sfc}(\lambda,\phi,t)$	surface pressure	(1.9)	hPa
R_b	bulk Richardson number	(1.23)	
$T(\lambda,\phi,\eta,t)$	absolute temperature	(1.9, 1.23)	K

Physical and meteorological constants

symbol	meaning	value
a	radius of the earth	$6.378_{10^6} m$
C_{pd}	specific heat of dry air at constant pressure	$1005.46 J\,kg^{-1}\,K^{-1}$
γ		$29.256 m\,K^{-1}$
ε	coefficient horizontal diffusion	$9000 m^2$
g	gravitational constant	$9.80665 m\,s^{-1}$
κ	von Karman constant	0.4

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