Space-Time Discretization of the CMAQ Vertical Advection-Diffusion Equation Using the Quasi-Analytic Method

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1. Introduction

A new approach is presented for calculating CMAQ 1-D advection and diffusion. This approach combines the separate CMAQ equations for 1-D advection and diffusion into one equation– the 1-D advection-diffusion partial differential equation– and combines the numerical and analytic approaches used to discretize this equation into a single discretization method–the Quasi-Analytic Method (QAM). QAM accommodates large timesteps (much larger than the CFL explicit timestep), hence fewer time-steps per unit of simulation time, without significant loss of accuracy. This characteristic of QAM was the primary factor driving the method's development.

The QAM has two flavors — Spatial-QAM (S-QAM) and Temporal-QAM (T-QAM).The S-QAM is used to spatially discretize the vertical advection-diffusion equation. The T-QAM is used to temporally discretize the ordinary differential equations that arise from using the S-QAM.

As part of developing the QAM, we needed to better define the upper and lower boundary conditions for the vertical advection-diffusion equation so that the calculations could proceed correctly. When using the QAM to derive the discretized equations, the equation for the upper layer automatically determines the appropriate type of boundary condition [upwind-like, specification of boundary concentration, or a mixture of the two, modified by vertical eddy diffusion] without a‘ priori assumptions.

Another side-effect of the QAM development has been the derivation of improved boundary conditions for chemical species concentrations at the top of the roughness layer. This should improve calculations above the roughness layer when strong vertical velocities occur near the top of this layer. The report [Herchenroder and Young 2006] contains detailed explanations of how the equations in this paper were derived and simplified.

2. Vertical Advection-Diffusion Equation

The CMAQ combined vertical advection-diffusion chemical species equation can be written as (see Byun and Ching 1999]) for the individual vertical-advection and vertical-diffusion equations)

$$\frac{\partial C}{\partial t} - \frac{\partial}{\partial z}\left(-\,w\,C + k\frac{\partial C}{\partial z}\right) = S \qquad (1)$$

where C, the molar mass concentration for chemical species i, w, the effective vertical velocity for species i, and S, the combined molar source function for this species are given by

$$\left.\begin{aligned} C &= (\widehat{\gamma})^{1/2}\,\rho\,m; \\ w &= w^{*} + k\,\left[\tfrac{1}{(\widehat{\gamma})^{1/2}\rho}\tfrac{\partial}{\partial z}\left((\widehat{\gamma})^{1/2}\,\rho\right)\right] \end{aligned}\right\} \qquad (2)$$

$$S = \frac{(\widehat{\gamma})^{1/2}\,\rho\,S^{*}}{\kappa};\;\; \kappa = 10^{-6}\frac{M}{M_{air}}\ , \qquad (3)$$

where t is time, z the vertical distance as measured from some convenient reference level,$\widehat{\gamma}$ the vertical Jacobian, ρ the atmospheric mass density, m the molar mixing ratio for species i in parts-per-million (related to q, the mixing ration for species i, by $q = \kappa\ m$ where κ is given by (3)), $w^{*} = w^{\dagger} - w_f$, $w^{\dagger}$ the vertical velocity, w_f the fall speed of species i, k the ver-

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tical diffusivity for that species, S^* the source function (units of q /sec) for species i, M the molecular weight of species i, M_{air} the molecular weight of air, and S^*/κ has units of parts-per-million per sec.

Equation (1) is the CMAQ advection-diffusion equation that will be discretized.

3. Spatially Discretize (1) Using the S-QAM

Decompose the atmosphere above the roughness layer into N_l layers. Consider layer j for $1 \le j \le N_l$. Let the index $[j-1/2,\ j,\ j+1/2]$ be associated with the [bottom, middle, top] of layer j respectively; $[z_{j-1/2},\ z_j\ , z_{j+1/2}]$ be the elevation at the [bottom, middle, top] of the layer respectively; and Δz_j be the thickness of the layer.

Consider layer j, for $j > 1$. (We consider layer $j = 1$ later). Define an integrating factor, $\Phi_j\left(z,t\right)$ and a length variable $\ell_j\left(z,t\right)$:

$$\Phi_j = \Phi_j\left(z,t\right) = \exp\left(-\int_{z_j}^{z} \frac{w\left(z',t\right)}{k\left(z',t\right)}\,dz'\right) \tag{4}$$

$$\ell_j = \ell_j\left(z,t\right) = \int_{z_j}^{z} \frac{\Phi_j\left(z',t\right)}{k\left(z',t\right)}\,dz' \tag{5}$$

Integrating (1) over layer j from $z_{j-1/2}$ to $z_{j+1/2}$ and rewriting the resulting equation in terms of Φ_j and ℓ_j, we have:

$$\left.\begin{array}{l} +\frac{\partial}{\partial t}\left(\int\limits_{z_{j-1/2}}^{z_{j+1/2}} C\,dz\right) \\ -\left(\frac{\partial(\Phi_j\,C)}{\partial \ell_j}\right)_{z_{j+1/2}} + \left(\frac{\partial(\Phi_j\,C)}{\partial \ell_j}\right)_{z_{j-1/2}} \end{array}\right\} = \int\limits_{z_{j-1/2}}^{z_{j+1/2}} S\,dz \tag{6}$$

Using the mean value theorem to evaluate integrals in (6) and simple divided differences to evaluate partial derivatives with respect to ℓ_j, (6) becomes

$$\left.\begin{array}{l} +\frac{\partial}{\partial t}\left(C_j\,\Delta z_j\right) \\ -\left(\frac{\Phi_j(z_{j+1},t)\,C_{j+1} - \Phi_j(z_j,t)\,C_j}{\Delta \ell_{j,j+1}}\right) \\ +\left(\frac{\Phi_j(z_j,t)\,C_j - \Phi_j(z_{j-1},t)\,C_{j-1}}{\Delta \ell_{j,j-1}}\right) \end{array}\right\} = S_j\,\Delta z_j \tag{7}$$

where, since $\ell_j\left(z_j,t\right) = 0$,

$$\left.\begin{array}{l} \Delta \ell_{j,j+1} = \ell_j\left(z_{j+1},t\right) - \ell_j\left(z_j,t\right) = \ell_j\left(z_{j+1},t\right) \\ \Delta \ell_{j,j-1} = \ell_j\left(z_j,t\right) - \ell_j\left(z_{j-1},t\right) = -\ell_j\left(z_{j-1},t\right) \end{array}\right\} \tag{8}$$

and where $C_j = C\left(z_j,t\right)$, $S_j = S\left(z_j,t\right)$, $C_{j-1} = C\left(z_{j-1},t\right)$, $C_{j+1} = C\left(z_{j+1},t\right)$.

Substituting (8) into (7), using the definitions of S_j, C_{j-1}, C_j, and C_{j+1} at the end of the previous paragraph, and then combining terms and simplifying, (7) can be expressed as:

$$\frac{\partial C_j}{\partial t} + L_j\,C_j = P_j \tag{9}$$

$$\left.\begin{array}{l} L_j = \frac{F_{j-1/2} + F_{j+1/2}}{\Delta z_j} \\ P_j = \frac{G_{j-1/2}}{\Delta z_j}\,C_{j-1} + \frac{G_{j+1/2}}{\Delta z_j}\,C_{j+1} \end{array}\right\} \tag{10}$$

where $F_{j+1/2} = \left[\ell_j\left(z_{j+1},t\right)\right]^{-1}$, $F_{j-1/2} = \left|\ell_j\left(z_{j-1},t\right)\right|^{-1}$, $G_{j+1/2} = \Phi_j\left(z_{j+1},t\right)\,F_{j+1/2}$, $G_{j-1/2} = \Phi_j\left(z_{j-1},t\right)\,F_{j-1/2}$.The right sides of $F_{j+1/2}$, $F_{j-1/2}$,$G_{j+1/2}$, and $G_{j-1/2}$ are evaluated in Appendix A of [Herchenroder and Young 2006].

Equation (9) is the S-QAM discretized form of (1). We will discretize (9) in time using the T-QAM to generate a space/time discretized equation for each layer of the model atmosphere except the lowest and highest one.

4. Discretize (9) in Time using the T-QAM

With the spatial discretization settled,we need to derive the corresponding temporally discretized equation using T-QAM. To apply the T-QAM to (9), we first approximate $L_j\left(t\right)$ and $P_j\left(t\right)$ as linearly interpolated functions of time over timestep $n+1$ of length Δt^{n+1}, that is, we let: $L_j\left(t\right) \approx L_j^n + \left(L_j^{n+1} - L_j^n\right)\left(t - t^n\right)\left[\Delta t^{n+1}\right]^{-1}$ and $P_j\left(t\right) \approx P_j^n + \left(P_j^{n+1} - P_j^n\right)\left(t - t^n\right)\left[\Delta t^{n+1}\right]^{-1}$where t^n is the time at the beginning of timestep $n+1$, t^{n+1} is the time at the end of the timestep, $\Delta t^{n+1} = t^{n+1} - t^n$, L_j^n, P_j^n are the values of L_j and P_j respectively at time-level $t = t^n$, and L_j^{n+1}, P_j^{n+1} the values of L_j and P_j, at time-level $t = t^{n+1}$. A superscript of n or $n+1$ on a variable means that the variable is evaluated at time-level t^n or t^{n+1} respectively. Sometimes we will refer to time-levels t^n or t^{n+1} as time-level n or time-level $n+1$ respectively.

Substituting the expressions for $L_j(t)$ and $P_j(t)$ into (9), and then solving the resulting differential equation analytically (see Appendix B of [Herchenroder and Young 2006] for details) for C_j^{n+1}, we find that:

$$C_j^{n+1} = \begin{cases} +C_j^n \exp\left(-\tau_j^{n+1}\right) \\ +B_j^{n+1} P_j^n + A_j^{n+1} P_j^{n+1} \end{cases} \tag{11}$$

$$\tau_j^{n+1} = \left(\Delta t^{n+1}/2\right) \left(L_j^n + L_j^{n+1}\right) \tag{12}$$

$$L_j = \left(F_{j-1/2} + F_{j+1/2}\right)/\Delta z_j \tag{13}$$

$$P_j = \begin{cases} +\frac{G_{j-1/2}}{\Delta z_j} C_{j-1} \\ +\frac{G_{j+1/2}}{\Delta z_j} C_{j+1} + S_j \end{cases} \tag{14}$$

where L_j^n is given by (13) evaluated at time-level n, P_j^n by (14) at that same time-level, L_j^{n+1} is given by (13) evaluated at time-level $n+1$, and P_j^{n+1} by (14) at that same time-level, Expressions for A_j^{n+1}**,** B_j^{n+1} in (11) are derived in Appendix B of [Herchenroder and Young 2006].

The final step in the T-QAM process for layers $j = 2, ..., (N_l-1)$ can now be taken. Substituting (14) into (11) and re-arranging terms produces the following spatial tri-diagonal equation for $j = 2, ..., (N_l - 1)$:

$$a_j^{n+1} C_{j-1}^{n+1} + C_j^{n+1} + c_j^{n+1} C_{j+1}^{n+1} = b_j^{n+1} \tag{15}$$

$$a_j^{n+1} = -A_j^{n+1} \left(G_{j-1/2}^{n+1}/\Delta z_j\right)$$

$$c_j^{n+1} = -A_j^{n+1} \left(G_{j+1/2}^{n+1}/\Delta z_j\right)$$

$$b_j^{n+1} = \begin{cases} +C_j^n \exp\left(-\tau_j^{n+1}\right) \\ +B_j^{n+1} P_j^n + A_j^{n+1} S_j^{n+1} \end{cases} \tag{16}$$

Equation (16) is appropriate for all layers except layer $j = 1$, right above the roughness layer, and layer $j = N_l$ at the top layer of the model atmosphere. For the top layer, we will use (15) **but** with C_{j+1}^{n+1} now being specified a half layer above the top boundary of the model atmosphere. In addition, we assume that, w_{N_l}, the effective vertical velocity for species i at the top of layer N_l, is non-zero in general. The difference equation for the uppermost layer is therefore given by:

$$a_{N_l}^{n+1} C_{N_l-1}^{n+1} + C_{N_l}^{n+1} = -c_{N_l}^{n+1} C_{g,(N_l+1)}^{n+1} + b_{N_l}^{n+1} \tag{17}$$

where the g subscript on the right side of (17) indicates that the concentration is specified as a boundary condition. This completes the derivation of the discretized equations for all layers but layer $j = 1$. Now consider that layer.

5. Dry-Deposition Boundary Condition

Before the difference equation for layer $j = 1$ can be derived, the dry-deposition boundary condition at the bottom of this layer, i.e. at $z = z_{1/2}$, must be specified. However, the specification of this condition is not trivial.The generalized boundary condition at the bottom of layer $j = 1$, is found to be (see Appendix C of [Herchenroder and Young 2006] for derivation):

$$-w_{1/2} C_{1/2} + \left(k\frac{\partial C}{\partial z}\right)_{z_{1/2}} = \begin{cases} +\Delta z_r \frac{\partial C_{1/2}}{\partial t} \\ +V_d C_{1/2} - S_a \end{cases} \tag{18}$$

$$\left.\begin{aligned} \Delta z_r &\approx \epsilon_r \left(z_{1/2} - z_{-1/2}\right) \\ S_a &= \frac{\left[(\widehat{\gamma})^{1/2}\rho\right]_{1/2} S_a^*}{\kappa} \end{aligned}\right\} \tag{19}$$

where a subscript of 1/2 on the variables w, C, k, $k\frac{\partial C}{\partial z}$,$(\widehat{\gamma})^{1/2}\rho$ denotes their value at $z = z_{1/2}$, V_d is the dry deposition velocity for species i at $z = z_{1/2}$, Δz_r is the effective thickness of the roughness layer, ϵ_r is a parameter < 1 (typically 0.1 to 0.25), $z = z_{-1/2}$ is the bottom of the roughness layer, $z_{1/2} - z_{-1/2}$ is the thickness of the roughness layer, S_a^* is the area source term for species i at $z = z_{1/2}$, and κ is a constant defined in (3).

The boundary condition, (18), is a generalization of one used at present in CMAQ [Byun and Ching 1999] and other air quality models. However, numerical experiments by showed that when $w_{1/2}$ is < 0 and large in magnitude, the traditional boundary condition induces unrealistically large values of $C_{1/2}$ and C_1. Hence the need for an improved boundary condition at the bottom of layer $j = 1$, namely. (18).

6. Derive Two Equations for Layer $j = 1$

Since there are two unknowns, C_1 and $C_{1/2}$, for layer $j = 1$, the lowest computational layer, there are two equations that must be derived for this layer. One equation is the vertically integrated, over layer $j = 1$, advection-diffusion equation. The second equation is the doubly vertically integrated, over layer $j = 1$, advection-diffusion equation. Summary of the derivations follows (see also Appendix H of [Herchenroder and Young 2006] for details).

a. Vertically Integrated Equation for Layer $j = 1$

Deriving the vertically integrated equation for layer $j = 1$ is done in a manner similar to the way we derived the S-QAM equations for the other layers. The only difference is the imposition of the boundary condition at the bottom of the layer. As a first approximation, we neglect terms multiplied by Δz_r, the effective thickness of the roughness layer. The resulting ordinary differential equation in time,

$$\left.\begin{array}{l} +\Delta z_1 \frac{\partial C_1}{\partial t} + V_d\, C_{1/2} \\ + F_{3/2}\, C_1 - G_{3/2}\, C_2 \end{array}\right\} = \left\{\begin{array}{l} +S_1\, \Delta z_1 \\ + S_a \end{array}\right. \tag{20}$$

relates C_1 and $C_{1/2}$ to each other and to C_2, which is the value of C near the center of layer $j = 2$. In (20), $C_1 = C(z_1, t)$, $S_1 = S(z_1, t)$, $C_2 = C(z_2, t)$, $\Delta z_1 = z_{3/2} - z_{1/2}$ is the thickness of layer $j = 1$, $F_{3/2}$ and $G_{3/2}$ are given by

$$\left.\begin{array}{l} F_{3/2} = \frac{1}{\ell_1(z_2,t)} \\ G_{3/2} = \frac{\Phi_1(z_2,t)}{\ell_1(z_2,t)} \end{array}\right\} \tag{21}$$

Integrating factor $\Phi_1(z, t)$ and length variable $\ell_1(z, t)$ for layer $j = 1$ are:

$$\Phi_1 = \Phi_1(z, t) = \exp\left(-\int_{z_1}^{z} \frac{w(z', t)}{k(z', t)}\, dz'\right) \tag{22}$$

$$\ell_1 = \ell_1(z, t) = \int_{z_1}^{z} \frac{\Phi_1(z', t)}{k(z', t)}\, dz' \tag{23}$$

The right sides of $F_{3/2}$ and $G_{3/2}$ in (21) are evaluated in Appendix A of [Herchenroder and Young 2006].

b. Doubly Vertically Integrated Equation

We need one more equation to relate $C_{1/2}$ and C_1 to each other. The derivation of this equation starts with the vertical advection-diffusion equation (1) and then doubly integrates it in the vertical over layer $j = 1$. The second integration is evaluated between the bottom of the layer and the gridpoint at $z = z_1$, near the middle of the layer. The partial derivative of C with respect to time t is neglected when doing the double vertical integration.

The resulting ordinary differential equation in time relates C_1 to $C_{1/2}$. More derivation details are given in Appendix H of [Herchenroder and Young 2006]. The doubly integrated equation is given approximately by:

$$(1 + J_d)\, C_{1/2} - \Phi'_{1/2}\, C_1 = \left\{\begin{array}{l} +J_0\, S_a \\ +J_1\, S_1 \end{array}\right. \tag{24}$$

$$\Phi_{1/2} = \Phi_{1/2}(z, t) = \exp\left(-\int_{z_{1/2}}^{z} \frac{w(z', t)}{k(z', t)}\, dz'\right) \tag{25}$$

$$\ell_{1/2} = \ell_{1/2}(z, t) = \int_{z_{1/2}}^{z} \frac{\Phi_{1/2}(z', t)}{k(z', t)}\, dz' \tag{26}$$

$$\left.\begin{array}{lcl} J_d & = & J_0\, V_d \\ \Phi'_{1/2} & = & \Phi_{1/2}(z_1, t) \end{array}\right\} \tag{27}$$

$$J_0 = J_0(t) = \ell_{1/2}(z_1, t) = \int_{z_{1/2}}^{z_1} \frac{\Phi_{1/2}(z, t)}{k(z, t)} dz\ ; \tag{28}$$

$$J_1 = J_1(t) = \int_{z_{1/2}}^{z_1} \frac{\Phi_{1/2}(z,t)}{k(z,t)} \left(z - z_{1/2}\right) dz; \quad (29)$$

with $\Delta z_{3/4} = z_1 - z_{1/2}$ being the distance between $z = z_{1/2}$, the bottom of layer $j = 1$, and $z = z_1$, the grid point near the middle of the layer.

The integral J_0 defined in (28) is evaluated in two steps; these are are documented in Appendices F and D of [Herchenroder and Young 2006]. The integral J_1 is expressed in terms of the integral J_0. The derivation of the expression for each integral is found in Appendix F of that reference.

Equation (24) is the S-QAM discretized second equation needed for layer $j = 1$. It is the last equation needed to close the system of equations for the $N_l + 1$ unknown concentrations $C_{1/2,}^{n+1}$, C_1^{n+1}, ..., $C_{N_l}^{n+1}$. Equations (20) and (24) must be discretized in time to generate the final two space-time discretized equations that are needed. Once these two equations have been temporally discretized, we will have $N_l + 1$ equations for $N_l + 1$ unknown concentrations.

c. Altrnate Form of Equations (20) and (24)

In order to not deviate too far from previous work in this initial paper presenting the QAM, an alternate form of (20) and (24) will be displayed and then discretized in time using the T-QAM.

Previous studies ([Byun and Ching 1999], [Findlayson-Pitts and Pitts 2000], [Jacobson 1999]) have used electrical analogues to model dry deposition related processes. The studies introduce equivalent resistences and we shall do so here. Equivalent resistences introduced below all include capital R. The alternate form of the two equations, in terms of equivalent resistences is:

$$\left.\begin{array}{l} +\frac{\partial C_1}{\partial t} + \frac{1}{\Delta z_1}\left(\frac{1}{R_d} C_{1/2} + F_{3/2}\, C_1\right) \\ -\frac{G_{3/2}}{\Delta z_1} C_2 \end{array}\right\} \approx \left\{\begin{array}{l} +S_1 \\ +\frac{S_a}{\Delta z_1} \end{array}\right. \quad (30)$$

$$C_{1/2} \approx R_d \left(\frac{C_1}{R_d^\dagger + R_A^\dagger} + S_1^\dagger\right) \quad (31)$$

$$\left.\begin{array}{l} R_d = \frac{1}{V_d};\; R_d^\dagger = \frac{R_d}{\Phi'_{1/2}}; \\ R_A = J_0;\; R_A^\dagger = \frac{R_A}{\Phi'_{1/2}}; \\ R_B = \frac{J_1}{\Delta z_1} \end{array}\right\} \quad (32)$$

$$S_1^\dagger = \left(R_A^*\right) S_a + \left(R_B^*\, \Delta z_1\right) S_1 \quad (33)$$

where $R_d^\dagger$, $R_A^\dagger$, R_d, R_A, and R_B are the equivalent resistances, $F_{3/2}$ and $G_{3/2}$ are given by (21), and

$$R_A^* = \frac{R_A}{R_d + R_A};\; R_B^* = \frac{R_B}{R_d + R_A};$$

We now substitute (31) into (30), thereby eliminating $C_{1/2}$ in favor of C_1. The resulting equation for C_1 is, after combining terms, simplifying, and expressing in equivalent resistence form, is:

$$\frac{\partial C_1}{\partial t} + L_1\, C_1 = P_1 \quad (34)$$

$$L_1 = L_1(t) = \frac{1}{\Delta z_1}\left(F_{3/2} + \frac{1}{R_d^\dagger + R_A^\dagger}\right) \quad (35)$$

$$P_1 = P_1(t) = \frac{G_{3/2}}{\Delta z_1} C_2 + \hat{S}_1 \quad (36)$$

$$\hat{S}_1 = R_d^* \frac{S_a}{\Delta z_1} + \left[1 - R_B^*\right] S_1$$

$$R_d^* = \frac{R_d}{R_d + R_A}$$

Equation 34 is the S-QAM equation for layer $j = 1$.

d. Discretize (34) Using the T-QAM

We now will discretize it in time using the T-QAM. Approximating $L_1(t)$ and $P_1(t)$ as linearly interpolated functions of time over timestep $n+1$ of length Δt^{n+1}, and then solving the resulting differential equation analytically for C_1^{n+1}, one finds that (see Appendix B of [Herchenroder and Young 2006] for derivation):

$$C_1^{n+1} = \left\{\begin{array}{l} +C_1^n \exp\left(-\tau_1^{n+1}\right) \\ +B_1^{n+1}\, P_1^n + A_1^{n+1}\, P_1^{n+1} \end{array}\right. \quad (37)$$

$$\tau_1^{n+1} = \frac{\Delta t^{n+1}}{2} \left(L_1^n + L_1^{n+1} \right) \tag{38}$$

L_1^n is given by (35) evaluated at time-level n, P_1^n by (36) at that same time-level, L_1^{n+1} is given by (35) evaluated at time-level $n+1$, and P_1^{n+1} by (36) at that same time-level, and A_1^{n+1}, B_1^{n+1} are given by A_j^{n+1} and B_j^{n+1} in Appendix B of [Herchenroder and Young 2006] but with $j = 1$, i.e.:

$$\left.\begin{array}{l} P_1^n = \frac{G_{3/2}^n}{\Delta z_1} C_2^n + \hat{S}_1^n \\ P_1^{n+1} = \frac{G_{3/2}^{n+1}}{\Delta z_1} C_2^{n+1} + \hat{S}_1^{n+1} \end{array}\right\} \tag{39}$$

Now substitute P_1^{n+1}, given in (39), into (37) and bring all terms involving C_2^{n+1} to the left side of (37). The resulting QAM discretized equation is:

$$C_1^{n+1} + c_1^{n+1} C_2^{n+1} = b_1^{n+1} \tag{40}$$

$$c_1^{n+1} = -A_1^{n+1} \frac{G_{3/2}^{n+1}}{\Delta z_1} \tag{41}$$

$$b_1^{n+1} = \left\{ \begin{array}{l} +C_1^n \exp\left(-\tau_1^{n+1}\right) \\ +B_1^{n+1} P_1^n + A_1^{n+1} \hat{S}_1^{n+1} \end{array} \right. \tag{42}$$

This completes the QAM derivation of the discretized coupled equations for layer $j = 1$.

7. Tri-diagonal Matrix Equation

Equation (42) for $j = 1$ must be solved simultaneously along with (17) for $j = N_l$ and (15) for $j = 2, 3, ..., (N_l - 1)$. Once the solution has been found, then the species concentrations can be found for each layer of the atmosphere at time-level t^{n+1}.

The N_l equations in the N_l unknowns represent a tri-diagonal matrix equation Once this equation has been solved, $C_{1/2}^{n+1}$ can be determined using (31), (32), and (33) evaluated at the time-level t^{n+1}.

The tri-diagonal matrix equation is solved using the Thomas Algorithm ([Byun and Ching 1999], Appendix 7A). However, to minimize numerically generated noise, it has been found that a three-step scaling process, and then an appropriate inverse-scaling process, must be used. The scaling and inverse-scaling process is described in Appendix G of [Herchenroder and Young 2006].

8. Numerical Implementation of QAM

Fortran 90 code was written to implement the QAM. The accuracy of the computed results was compared with an exact solution of a toy problem that had been developed. The toy problem consists of a constant vertical velocity, eddy diffusivity and dry deposition velocity. An exponentially damped (in the vertical), sinusoidally varying (in time), volume source function is assumed. A sinusoidally varying (in time) surface area source function is also assumed to exist at the top of the roughness layer.

A model atmosphere consisting of 200 layers was assumed for test purposes. The planetary boundary layer (PBL) consisted to 50 layers, each 20m thick. The free atmosphere above the PBL consisted of 150 layers, each 100m thick. The numerical solution used the exact solution at the top of the model as the boundary condition and the exact solution at the initial time as initial condition.A timestep of one hour was used. The explicit timestep for the model is 20 seconds. Note that the timestep is 180 times larger than the explicit timestep! The model was run for 48 model hours; no instabilities were encountered. During the 48 hour timespan, the computed solution differed less than 1% from the exact solutation at and above the middle of layer 1.

9. References

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