Example Calculations of AQMEII-4 Variables.

Example 1: Resistance model of Figure 2(a).

Table 2. AQMEII-4 reported gas deposition variables corresponding to the resistance model of Figure 2(a).

Name as described here	AQMEII-4 Variable Name	Formulae
r_a	RES-AERO	$RES\text{-}AERO = r_a$
r_c	RES-SURF	$RES\text{-}SURF = \left((r_{stom1} + r_{stom2} + r_m)^{-1} + (r_{cut1} + r_{cut2})^{-1} + (r_{soil1} + r_{soil2} + r_{soil3})^{-1}\right)^{-1}$
r_s	RES-STOM	$RES\text{-}STOM = r_{stom1} + r_{stom2}$
r_m	RES-MESO	$RES\text{-}MESO = r_m$
r_c	RES-CUT	$RES\text{-}CUT = r_{cut1} + r_{cut2}$
E_{STOM}	ECOND-ST	$ECOND\text{-}ST = \left(\frac{(r_{stom1}+r_{stom2}+r_m)^{-1}}{(r_{stom1}+r_{stom2}+r_m)^{-1}+(r_{cut1}+r_{cut2})^{-1}+(r_{soil1}+r_{soil2}+r_{soil3})^{-1}}\right) V_d$
E_{CUT}	ECOND-CUT	$ECOND\text{-}CUT = \left(\frac{(r_{cut1}+r_{cut2})^{-1}}{(r_{stom1}+r_{stom2}+r_m)^{-1}+(r_{cut1}+r_{cut2})^{-1}+(r_{soil1}+r_{soil2}+r_{soil3})^{-1}}\right) V_d$
E_{SOIL}	ECOND-SOIL	$ECOND\text{-}SOIL = \left(\frac{(r_{soil1}+r_{soil2}+r_{soil3})^{-1}}{(r_{stom1}+r_{stom2}+r_m)^{-1}+(r_{cut1}+r_{cut2})^{-1}+(r_{soil1}+r_{soil2}+r_{soil3})^{-1}}\right) V_d$
E_{LCAN}	ECOND-LCAN	$ECOND\text{-}LCAN = -9$ $(not\ included\ as\ a\ separate\ deposition\ pathway)$
$r_{b,\ stom}$	RES-QLST	$RES\text{-}QLST = r_b\ assuming\ r_{stom1} is\ the\ stomatal\ pathway\ quasi-laminar\ sublayer\ resistance$
$r_{b,cut}$	RES-QLCT	$RES\text{-}QLCT = r_{cut1}, assuming\ r_{cut1} is\ the\ cuticle\ pathway\ quasi-laminar\ sublayer\ resistance$
$r_{b,soil}$	RES-QLSL	$RES\text{-}QLCL = r_{soil1}, assuming\ r_{soil1} is\ the\ soil\ pathway\ quasi-laminar\ sublayer\ resistance$
$r_{b,lcan}$	RES-QLLC	$RES\text{-}QLLC = -9\ (lower\ canopy\ deposition\ pathway\ is\ not\ included\ in\ this\ deposition\ model)$
r_{dc}	RES-CONV	$RES\text{-}CONV = -9\ (lower\ canopy\ deposition\ pathway\ is\ not\ included\ in\ this\ deposition\ model)$

Comments: This deposition network does not have a separate resistance for lower canopy buoyant convection or a deposition pathway to exposed surfaces, hence the associated effective conductance and QSLB term cannot be reported.

Example 3: Resistance model of Figure 2(b).

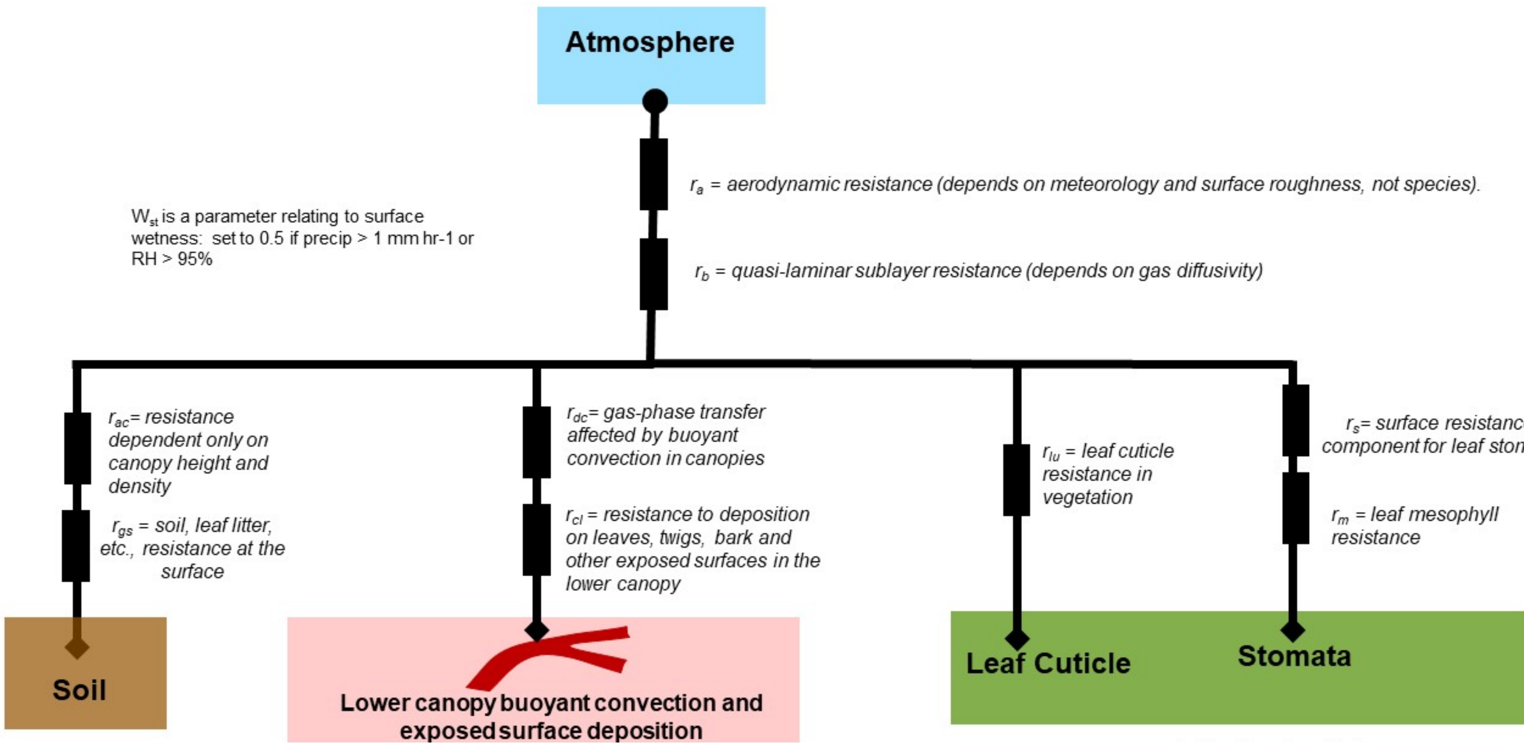
Table 3. AQMEII-4 reported gas deposition variables corresponding to the resistance model of Figure 2(b).

Name as described here	AQMEII-4 Variable Name	Formulae
r_a	RES-AERO	$RES\text{-}AERO = r_a$
r_c	RES-SURF	$RES\text{-}SURF = ((r_s + r_m)^{-1} + (r_{lu})^{-1} + (r_{soil1} + r_{soil2})^{-1})^{-1}$
r_s	RES-STOM	$RES\text{-}STOM = r_s$
r_m	RES-MESO	$RES\text{-}MESO = r_m$
r_c	RES-CUT	$RES\text{-}CUT = r_{lu}$
E_{STOM}	ECOND-ST	$ECOND\text{-}ST = \left(\frac{(r_s+r_m)^{-1}}{(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{soil1}+r_{soil2})^{-1}}\right) V_d$
E_{CUT}	ECOND-CUT	$ECOND\text{-}CUT = \left(\frac{(r_{lu})^{-1}}{(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{soil1}+r_{soil2})^{-1}}\right) V_d$
E_{SOIL}	ECOND-SOIL	$ECOND\text{-}SOIL = \left(\frac{(r_{soil1}+r_{soil2})^{-1}}{(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{soil1}+r_{soil2})^{-1}}\right) V_d$
E_{LCAN}	ECOND-LCAN	$ECOND\text{-}LCAN = -9$ $(not\ included\ as\ a\ separate\ deposition\ pathway)$
$r_{b,\ stom}$	RES-QLST	$RES\text{-}QLST = r_b$
$r_{b,cut}$	RES-QLCT	$RES\text{-}QLCT = r_b$
$r_{b,soil}$	RES-QLSL	$RES\text{-}QLSL = r_b$
$r_{b,lcan}$	RES-QLLC	$RES\text{-}QLLC = -9$ $(lower\ canopy\ deposition\ pathway\ is\ not\ included\ in\ this\ deposition\ model$
r_{dc}	RES-CONV	$RES\text{-}CONV = -9$ $(lower\ canopy\ deposition\ pathway\ is\ not\ included\ in\ this\ deposition\ model$

Example 4: GEM-MACH model.

These are the calculations for the Environment and Climate Change Canada model GEM-MACH (Global Environmental Multiscale- Modelling Air-quality and CHemistry). The resistance diagram for this model is shown in Figure 3. The deposition algorithm closely follows Wesely's original, hence the similarities to Figure 1. In GEM-MACH, snow, when present, is treated as a separate land use type.

Figure 3. Resistance diagram for the ECCC GEM-MACH model.



The main difference between the resistances in Wesely (1989) and the GEM-MACH resistances is the addition of a surface wetness term, (1-Wst), intended to account for the presence of wet surfaces.

Table 4. Example 3: AQMEII-4 reported gas deposition variables corresponding to the GEM-MACH resistance model of Figure 3.

Name as described here	AQMEII-4 Variable Name	Formulae
r_a	RES-AERO	$RES\text{-}AERO = r_a$
r_c	RES-SURF	$RES\text{-}SURF = \left((1 - W_{st})(r_s + r_m)^{-1} + (r_{lu})^{-1} + (r_{dc} + r_{cl})^{-1} + \left(r_{ac} + r_{gs}\right)^{-1}\right)^{-1}$
r_s	RES-STOM	$RES\text{-}STOM = r_s$
r_m	RES-MESO	$RES\text{-}MESO = r_m$
r_c	RES-CUT	$RES\text{-}CUT = r_{lu}$
E_{STOM}	ECOND-ST	$ECOND\text{-}ST= \left(\frac{(1-W_{st})(r_s+r_m)^{-1}}{(1-W_{st})(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+\left(r_{ac}+r_{gs}\right)^{-1}}\right) V_d$
E_{CUT}	ECOND-CUT	$ECOND\text{-}CUT = \left(\frac{(r_{lu})^{-1}}{(1-W_{st})(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+\left(r_{ac}+r_{gs}\right)^{-1}}\right) V_d$
E_{SOIL}	ECOND-SOIL	$ECOND\text{-}SOIL= \left(\frac{(r_{dc}+r_{cl})^{-1}}{(1-W_{st})(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+\left(r_{ac}+r_{gs}\right)^{-1}}\right) V_d$
E_{LCAN}	ECOND-LCAN	$ECOND\text{-}LCAN = \left(\frac{(r_{dc}+r_{cl})^{=1}}{(1-W_{st})(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+\left(r_{ac}+r_{gs}\right)^{-1}}\right) V_d$
$r_{b,\ stom}$	RES-QLST	$RES\text{-}QLST = r_b$
$r_{b,cut}$	RES-QLCT	$RES\text{-}QLCT = r_b$
$r_{b,soil}$	RES-QLSL	$RES\text{-}QLSL = r_b$
$r_{b,lcan}$	RES-QLLC	$RES\text{-}QLLC = r_b$
r_{dc}	RES-CONV	$RES\text{-}CONV= r_{dc}$

Example 4: CMAQ.

The second specific air-quality model example is the algorithm used by the US EPA's Community Multiscale Air Quality (CMAQ) model. In this particular case, separate branches occur for the vegetated versus non-vegetated fraction within each model grid cell, and further branching resistance pathways take into account the fraction of the grid cell which is wet versus dry, and snow-covered versus non-snow covered. In-canopy convective effects are only calculcated for in the vegetated fraction.

Figure 4. Resistance diagram for the US EPA CMAQ model.

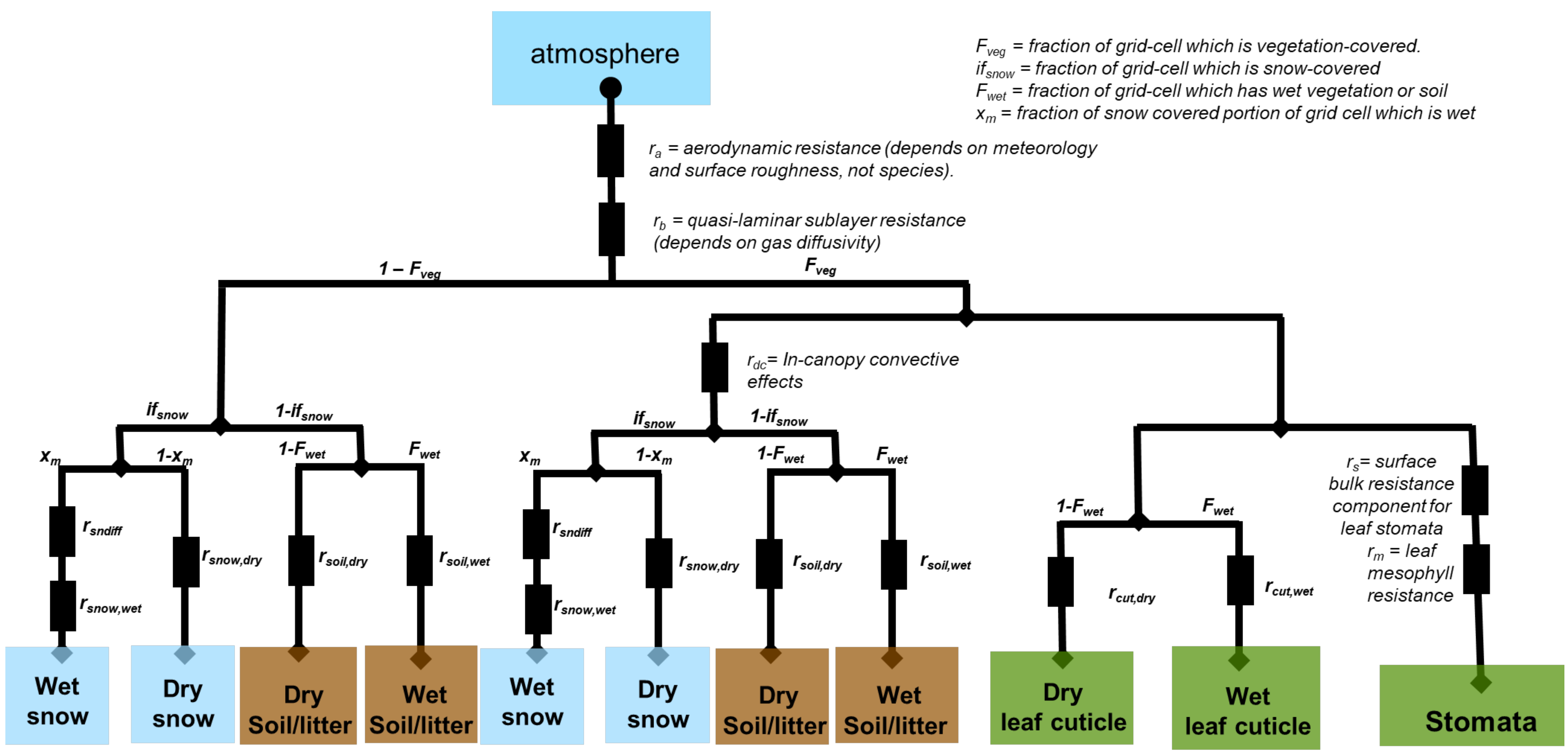


Table 5. AQMEII-4 reported gas deposition variables corresponding to the CMAQ resistance model of Figure 4.

Name as described here	AQMEII-4 Variable Name	Formulae
r_a	RES-AERO	$RES\text{-}AERO = r_a$
r_c	RES-SURF	$RES\text{-}SURF = \left\{ F_{veg}\left(\frac{1}{r_s+r_m}+\frac{(1-F_{wet})LAI}{r_{cut,dry}}+\frac{F_{wet}*LAI}{r_{cut,wet}}+\frac{1}{r_{dc}+\frac{1}{(1-ifsnow)\left(\frac{(1-F_{wet})}{r_{soil,dry}}+\frac{F_{wet}}{r_{soil,wet}}\right)+(ifsnow)\left(\frac{(1-x_m)}{r_{snow,dry}}+\frac{x_m}{r_{sndiff}+r_{snow,wet}}\right)}}\right) + (1-F_{veg})\left((1-ifsnow)\left(\frac{(1-F_{wet})}{r_{soil,dry}}+\frac{F_{wet}}{r_{soil,wet}}\right)+(ifsnow)\left(\frac{(1-x_m)}{r_{snow,dry}}+\frac{x_m}{r_{sndiff}+r_{snow,wet}}\right)\right)\right\}^{-1}$
r_s	RES-STOM	$RES\text{-}STOM = \frac{r_s}{F_{veg_S}}$
r_m	RES-MESO	$RES\text{-}MESO = \frac{r_m}{F_{veg}}$
r_c	RES-CUT	$RES\text{-}CUT = \left[F_{veg}\left(\frac{(1-F_{wet})LAI}{r_{cut,dry}}+\frac{F_{wet}*LAI}{r_{cut,wet}}\right)\right]^{-1}$
E_{STOM}	ECOND-ST	$ECOND\text{-}ST = \left[\frac{(F_{veg})}{(r_s+r_m)}\right](RES-SURF)\,V_d$
E_{CUT}	ECOND-CUT	$ECOND\text{-}CUT = \left[F_{veg}\left(\frac{(1-F_{wet})LAI}{r_{cut,dry}}+\frac{F_{wet}LAI}{r_{cut,wet}}\right)\right](RES-SURF)V_d$
E_{SOIL}	ECOND-SOIL	$ECOND\text{-}SOIL = \left[(1-F_{veg})\left((1-ifsnow)\left(\frac{(1-F_{wet})}{r_{soil,dry}}+\frac{F_{wet}}{r_{soil,wet}}\right)+(ifsnow)\left(\frac{(1-x_m)}{r_{snow,dry}}+\frac{x_m}{r_{sndiff}+r_{snow,wet}}\right)\right)\right](RES-SURF)\,V_d$
E_{LCAN}	ECOND-LCAN	$ECOND\text{-}LCAN = \left[\frac{F_{veg}}{r_{dc}+\frac{1}{(1-ifsnow)\left(\frac{(1-F_{wet})}{r_{soil,dry}}+\frac{F_{wet}}{r_{soil,wet}}\right)+(ifsnow)\left(\frac{(1-x_m)}{r_{snow,dry}}+\frac{x_m}{r_{sndiff}+r_{snow,wet}}\right)}}\right](RES-SURF)\,V_d$
$r_{b,\,stom}$	RES-QLST	$RES\text{-}QLST = r_b$
$r_{b,cut}$	RES-QLCT	$RES\text{-}QLCT = r_b$
$r_{b,soil}$	RES-QLSL	$RES\text{-}QLSL = r_b$
$r_{b,lcan}$	RES-QLLC	$RES\text{-}QLLC = r_b$
r_{dc}	RES-CONV	$RES\text{-}CONV = r_{dc}$

Note that the vegetated fraction used in the above equations for CMAQ is across all vegetation types: the quantities in Table 5 will be reported for each of the 15 generic land use categories for AQMEII-4. Note that the lower canopy pathway has been identified as such due to the presence of the rdc term; i.e. this points to its similarity with Wesely's original lower canopy pathway.

Example 5. Nemitz bidirectional flux model.

The final example is for the bidirectional flux model of Nemitz, used within CMAQ for ammonia gas fluxes. The model depends on three compensation point concentrations of gaseous ammonia, calculated for each branch of the three branches shown in Figure 5. While these influence the net deposition rate, the individual resistances and resistance pathways may be reported in the same fashion as the other examples (see Table 6). Note that there is some ambiguity in the effective conductances, in that a single "soil" pathway appears in this model. Here, it has been included under the "lower canopy" effective conductance, rather than the "soil" pathway of Wesely(1989), due to the presence of the r_{dc} term.

Figure 5. Nemitz bi-directional flux model for NH_3.

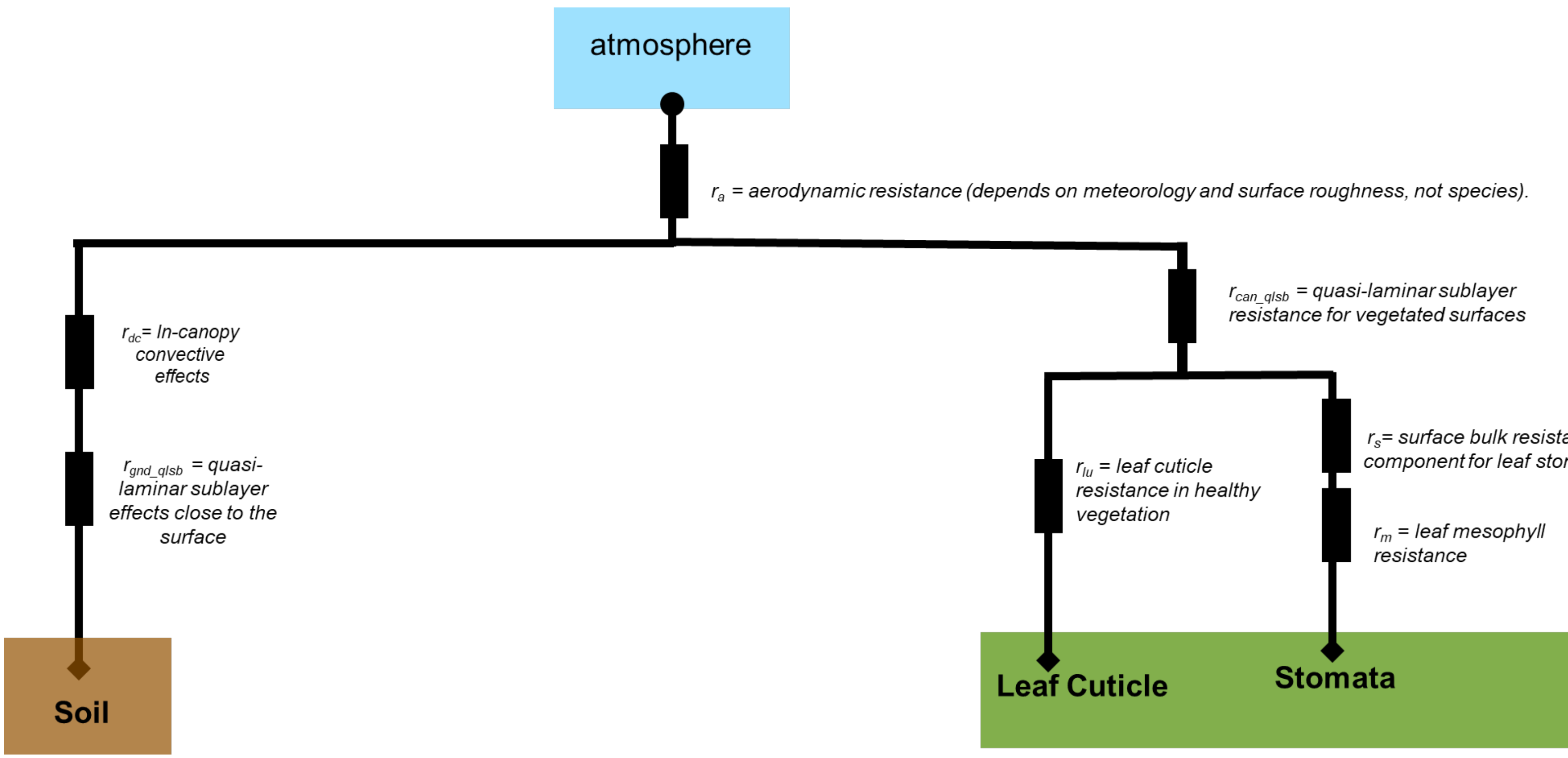


Table 6. Example 5: AQMEII-4 reported gas deposition variables corresponding to the Nemitz resistance model of Figure 5.

Name as described here	AQMEII-4 Variable Name	Formulae
r_a	RES-AERO	$RES\text{-}AERO = r_a$
r_c	RES-SURF	$RES\text{-}SURF = \left(\left(r_{can\_qlsb} + ((r_s + r_m)^{-1} + (r_{lu})^{-1})^{-1}\right)^{-1} + \left(r_{dc} + r_{gnd\_qlsb}\right)^{-1}\right)^{-1}$
r_s	RES-STOM	$RES\text{-}STOM = r_s$
r_m	RES-MESO	$RES\text{-}MESO = r_m$
r_c	RES-CUT	$RES\text{-}CUT = r_{lu}$
E_{STOM}	ECOND-ST	$ECOND\text{-}ST = \left(\frac{(r_s+r_m)^{-1}}{\left(r_{can\_qlsb}+((r_s+r_m)^{-1}+(r_{lu})^{-1})^{-1}\right)^{-1}+\left(r_{dc}+r_{gnd\_qlsb}\right)^{-1}}\right)V_d$
E_{CUT}	ECOND-CUT	$ECOND\text{-}CUT = \left(\frac{(r_{lu})^{-1}}{\left(r_{can\_qlsb}+((r_s+r_m)^{-1}+(r_{lu})^{-1})^{-1}\right)^{-1}+\left(r_{dc}+r_{gnd\_qlsb}\right)^{-1}}\right)V_d$
E_{SOIL}	ECOND-SOIL	$ECOND\text{-}SOIL = -9$ $(not\ included\ as\ a\ separate\ deposition\ pathway)$
E_{LCAN}	ECOND-LCAN	$ECOND\text{-}LCAN = \left(\frac{\left((r_{dc}+r_{gnd\_qlsb})\right)^{-1}}{\left(r_{can\_qlsb}+((r_s+r_m)^{-1}+(r_{lu})^{-1})^{-1}\right)^{-1}+\left(r_{dc}+r_{gnd\_qlsb}\right)^{-1}}\right)V_d$
$r_{b,\ stom}$	RES-QLST	$RES\text{-}QLST = r_{can\_qlsb}$
$r_{b,cut}$	RES-QLCT	$RES\text{-}QLCT = r_{can\_qlsb}$
$r_{b,soil}$	RES-QLSL	$RES\text{-}QLSL = r_{gnd\_qlsb}$
$r_{b,lcan}$	RES-QLLC	$RES\text{-}QLLC = -9$ $(lower\ canopy\ deposition\ pathway\ is\ not\ included\ in\ this\ deposition\ model$
r_{dc}	RES-CONV	$RES\text{-}CONV = r_{dc}$

In the above example, note that the branch containing the r_{dc} term has been designated as the lower canopy pathway, due to the presence of the canopy buoyant convection term r_{dc} (i.e. closest analogy to Wesely's setup is to have the pathway involving deposition to "soil" pathway is designated as a "lower canopy" pathway).

Bi-directional ammonia fluxes (TSD's ending in -292):

If a bidirectional flux algorithm for ammonia is employed in the model, then the flux may be either downwards (defined positive here) or upwards (defined negative, here). The generic equation for the bidirectional flux with this directionality is:

$$F_T = \frac{c_a - c_c}{r_{sum}} \tag{7}$$

Where F_T is the net flux, c_a and c_c are the atmospheric and canopy compensation point concentrations of ammonia gas, and r_{sum} is a sum of resistances. Different sources in the literature make use of different formula for both cc and rsum. For example, Zhang et al (2010) employs:

$$\begin{gathered} r_{sum} = r_a + r_b, and \\ c_c = \frac{\frac{c_a}{r_a + r_b} + \frac{c_s}{r_s} + \frac{c_g}{\boldsymbol{r_{ac}} + \boldsymbol{r_{gs}}}}{(r_a + r_b)^{-1} + (r_s)^{-1} + (\boldsymbol{r_{ac}} + \boldsymbol{r_{gs}})^{-1} + (r_{lu})^{-1}} \end{gathered} \tag{8}$$

Where c_s and c_g are compensation point concentrations relative to stomata and ground, respectively, and all other terms are defined as above. Pleim et al (2010) use:

$$\begin{gathered} r_{sum} = r_a + 0.5\, r_{inc} \\ r_{inc} = 14LAI\,\frac{h_{can}}{u_*} \\ c_c = \frac{-B + (B^2 - 4AC)^{0.5}}{2A} \end{gathered} \tag{9}$$

Where

$$\begin{gathered} A = r_{wet} G_t \\ B = r_{wb} G_t + LAI(1 - f_{wet}) - r_{wet}(G_a c_a + G_{sb} c_s + G_g c_g) \\ C = -r_{wb}(G_a c_a + G_{sb} c_s + G_g c_g) \end{gathered} \tag{10}$$

And

$$
\begin{gathered}
G_a = (r_a + 0.5 r_{inc})^{-1} \\
G_{sb} = (r_s + r_b)^{-1} \\
G_g = \left(r_{bg} + 0.5 r_{inc} + r_{soil}\right)^{-1} \\
G_t = G_{sb} + G_g + G_a + f_{wet} G_{cw} \\
G_{cw} = \frac{LAI}{r_b + r_{wet}} \\
r_{wet} = \frac{R_{wo}}{H_{eff}} \\
r_{wb} = r_{wet} + LAI\left[a_h\left(1 - f_{RH_s}\right) + r_b\right]
\end{gathered} \tag{11}
$$

Where the terms r_{soil}, H_{eff}, a_h, f_{RHs}, and R_{wo} are defined in Pleim *et al.* (2013). Note that in the latter reference (their equation (20)), the summation term in (10) above $G_a c_a$ is repeated twice within the bracketed terms (i.e. $\left(G_a c_a + G_{sb} c_s + G_g c_g\right)$ as above is written $\left(G_a c_a + G_{sb} c_s + G_a c_a + G_g c_g\right)$, but this second repeat is likely a typo).

Comparing approaches (8) versus (9 through 11), it can be seen that r_{sum}, r_a, and c_c are held in common by both approaches, and both approaches also make use of a stomatal (c_s) and ground (c_g) compensation point concentration, although how these terms are combined varies considerably between these two approaches. For this reason, these common terms are reported as a separate TSD for ammonia bi-directional fluxes in AQMEII-4 in order to allow cross-comparison of different approaches.

Table 7. Variables for bidirectional fluxes of ammonia.

Name as described here	AQMEII-4 Variable Name	Details
r_{sum}	RES-SUM-NH3	Net bi-directional flux ammonia resistance
r_a	RES-AERO-NH3	Net Aerodynamic resistance used for ammonia bi-directional fluxes
c_a	CONC-NH3-AIR	Air concentration of ammonia used for bi-directional flux calculations
c_c	COMP-NH3-NET	Net Ammonia Overall Compensation point concentration
c_g	COMP-NH3-GND	Net Ammonia Compensation point concentration with respect to ground
c_s	COMP-NH3-STO	Net Ammonia Compensation point concentration with respect to stomata

Note that the net flux of ammonia F_T appears as DFLUX-NH3 in the TSDs, and may be positive or negative depending on direction. Ammonia values for r_b, net canopy resistance, stomatal resistance, mesophyll resistance, cuticle resistance and the three effective conductances also appear elsewhere in the TSDs, both for the net land use and by AQMEII-4 land use category.

References:

Pleim, J.E., Bash, J.O., Walker, J.T., Cooter, E.J., Development and evaluation of an ammonia bidirectional flux parameterization for air quality models, J. Geophys. Res. Atm., 118, 3794-3806, 2013.

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