Derived Gas-Phase Deposition Velocity Parameters for AQMEII-4.

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Part of the proposed set of variables to be delivered under the AQMEII-4 protocol includes additional model outputs designed to allow process-oriented intercomparison between the different gas-phase deposition modules used in the participating regional air-quality models. These variables to be reported must be chosen with care, since the manner in which different deposition terms are formulated varies between the models.

We start with a description of one of the earliest literature examples using the "resistance" concept, and follow with both generic and specific examples as a guide to the AQMEII-4 participant. The special case of bidirectional fluxes of ammonia appears at the end of this document.

Deposition models are based on a resistance approach – Figure 1 shows an example for the scheme of Wesely (1989).

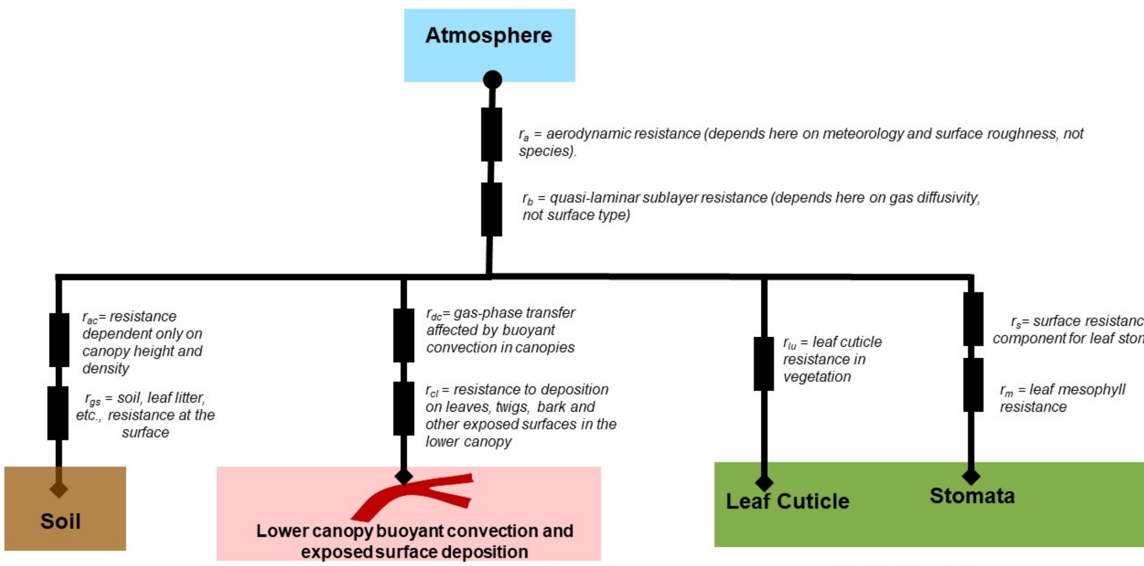


Figure 1. Gas-phase deposition velocity resistance diagram for the Wesely (1989) scheme.

In Figure 1, the components of the deposition velocity are described as specific process-based resistances to deposition, which are added in series for processes operating on the same depositional pathway, and in parallel when multiple surfaces for deposition exist. In Wesely's original formulation, four different deposition surfaces (i.e. deposition pathways) were proposed, not all of which have been retained in some subsequent models: soil, lower canopy and exposed surfaces, leaf cuticles, and plant stomata. All depositing gases are impeded by an aerodynamic resistance to deposition (r_a), which in Wesely (1989) depends on meteorology and surface roughness (but not on the properties of the gas being deposited), a quasi-laminar sublayer resistance (r_b) which in Wesely (1989) depends on the diffusion properties of the gas, and a bulk surface resistance term (r_c) composed of all of the parallel summation of the resistances associated with the processes specific to the surfaces upon which deposition occurs. The net deposition velocity for the gas is given by the series addition of r_a, r_b, and r_c:

$$\boldsymbol{v_d = (r_a + r_b + r_c)^{-1}} \tag{1}$$

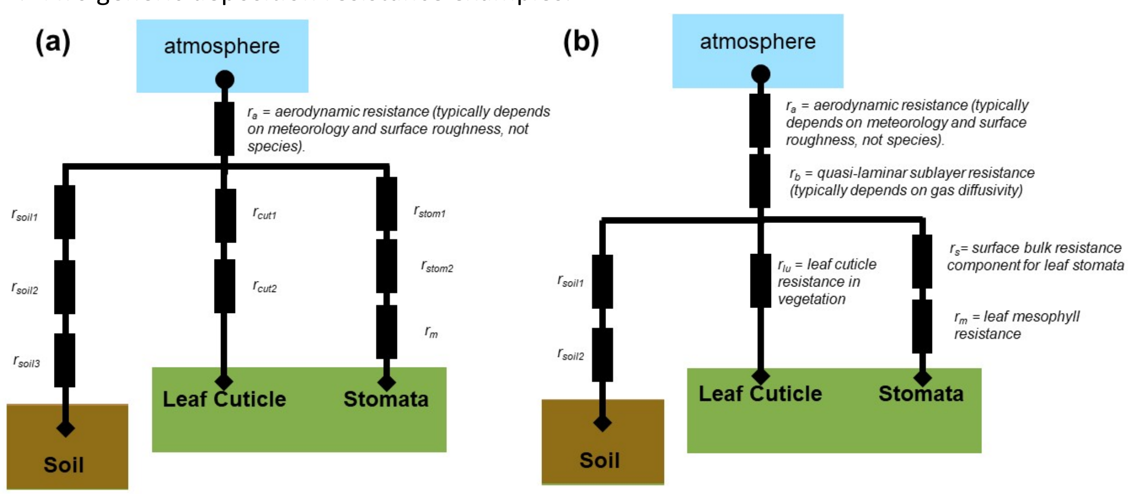
The bulk surface resistance in Wesely's formulation is given by the parallel addition of terms associated with the resistance to deposition of each pathway to a depositing surface:

$$\boldsymbol{r_c = \left((r_s + r_m)^{-1} + (r_{lu})^{-1} + (r_{dc} + r_{cl})^{-1} + \left(r_{ac} + r_{gs}\right)^{-1}\right)^{-1}} \tag{2}$$

The deposition velocity has units of m s^{-1}, and the resistances have the inverse units of s m^{-1}.

Work subsequent to Wesely (1989) has made use of the resistance approach, but with sometimes considerable variation in the resistance framework and number of depositing surfaces, and of the processes represented by individual resistances themselves. Two generic examples are shown in Figure 2.

Figure 2. Two generic deposition resistance examples.



In the examples of Figure 2, Wesely's deposition pathway for "lower canopy buoyancy and exposed surfaces" deposition has been neglected. The example of Figure 2 (a) also lacks a quasi-laminar sublayer resistance r_b applied across all surface types, however, this effect of r_b is included in a *surface-specific* sense (i.e. through r_{soil1}, r_{cut1}, r_{stom1}). These examples demonstrate the variety of ways in which processes are represented has diverged subsequent to Wesely's original resistance concept.

Despite the differences in resistance networks between different models, their deposition pathways may be compared using a concept we will refer to here as *effective conductance.* A conductance is simply the inverse of of resistance. An *effective* conductance is the contribution of a given depositional pathway to the deposition velocity in the same units as the deposition velocity. The sum of the effective conductances for all deposition pathways is the deposition velocity.

The effective conductances of the soil, lower canopy, cuticle and stomata branches specifically for Wesely (1989) are given by[1]:

$$E_{SOIL} = \left(\frac{(r_{ac}+r_{gs})^{-1}}{(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+(r_{ac}+r_{gs})^{-1}}\right)\boldsymbol{V_d} \tag{3}$$

$$E_{LCAN} = \left(\frac{(r_{dc}+r_{cl})^{-1}}{(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+(r_{ac}+r_{gs})^{-1}}\right)\boldsymbol{V_d} \tag{4}$$

$$\boldsymbol{E_{CUT}} = \left(\frac{(r_{lu})^{-1}}{(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+(r_{ac}+r_{gs})^{-1}}\right)\boldsymbol{V_d} \tag{5}$$

$$\boldsymbol{E_{STOM}} = \left(\frac{(r_s+r_m)^{-1}}{(r_s+r_m)^{-1}+(r_{lu})^{-1}+(r_{dc}+r_{cl})^{-1}+(r_{ac}+r_{gs})^{-1}}\right)\boldsymbol{V_d} \tag{6}$$

The denominator in each of equations (3) to (6) is the inverse of the bulk surface resistance r_c, while the numerators are the inverses of the resistances associated with each pathway of the bulk surface resistance. Note that the equations are specifically for the Wesely (1989) dry deposition resistance network, and require modification for other networks (several examples for different deposition modules appear as examples later in this document). We emphasize that the calculation of the effective conductances will depend on the resistance framework used, and require either post-processing calculation from all of the component resistances of the bulk surface resistance for a given framework, or on-line calculation during a model simulation. The effective conductances are an invaluable tool to determine which the deposition pathways for surface resistance drive spatiotemporal variability and inter-model differences in dry deposition, and to determine the extent to which each pathway impacts the net dry deposition. They also allow a cross-comparison of the main surface resistance pathways to be compared across different modelling frameworks, a key part of AQMEII-4.

In addition to the effective conductances for each depositional pathway, participants are asked to archive specific resistance terms held in common by most models. The latter were chosen based on the common or at least frequent use of a single resistance term to describe a specific deposition process, and are intended to allow a more detailed intercomparison within some of the deposition pathways.

[1] Note that the depositing molecules in each pathway in this example are influenced by the r_a and r_b terms prior to encountering the different surface resistance pathways, hence the fractional contributions of the four conductance pathways towards net deposition are exact, despite the fractions in the formula not including r_a and r_b explicitly. Some models include surface-specific quasi-laminar sublayer resistance terms; when this is the case, these terms appear in the definitions of effective conductance for that given model. Several example formulae for different resistance frameworks appear later in this document.

These resistances include:

(1) A species-independent aerodynamic resistance term, r_a.
(2) The bulk resistance to deposition associated with surfaces r_c.
(3) A term or series addition set of terms describing the net stomatal resistance, r_s.
(4) A term or series addition set of terms describing the net mesophyll resistance r_m.
(5) A term or series addition set of terms describing the net cuticle resistance, r_c.
(6) Terms to describe quasi-laminar sublayer resistance.
With regards to the quasi-laminar sublayer resistance: the implementation of quasi-laminar sublayer resistance (r_b in Wesely (1989)) differs between the different models. Some models making use of Wesely's original concept of a surface-independent term as per Figure 1. Others make use of quasi-laminar sublayer resistances as deposition pathway dependent (and hence surface-dependent) resistances as per Figure 2(a), where, for example, the r_{soil1}, r_{cut1}, and r_{stom1} terms could all potentially represent a quasi-laminar sublayer resistance, for each of the soil, cuticle and stomatal conductance pathways. The quasi-laminar sublayer resistance is thus to be reported in AQMEII-4 for each pathway – those models for which the term is independent of surface would report the same number for each of the four pathways, and these terms are designated "not present" (i.e given a value of -9) only if the given pathway does not exist in a deposition framework.
(7) A term to describe within-canopy buoyant convection, r_{dc}. Note that models which include a single deposition pathway to soil which incorporates r_{dc} should report that pathway as "lower canopy", not "soil", due to the greater degree of similarity of the pathway to Wesely's original "lower canopy" pathway due to r_{dc}'s inclusion.

Specific resistance terms for the soil deposition pathway and the lower canopy pathway have *not* been requested, since the implementation of these terms vary considerably between deposition models. For example, Wesely (1989) made use of a single term for the soil resistance (Fig. 1), while other deposition models may make use of two or three terms added in series (Fig. 2). Rather than request that these series summations within the soil and lower canopy pathways be reported, we note that they may be recovered from the reported effective conductances, deposition velocities, bulk surface resistances, and quasi-laminar sublayer resistances, if desired.

For AQMEII-4, the following terms are to be reported for each of the gases SO_2, NO_2, NO, HNO_3, NH_3, PAN, HNO_4, N_2O_5, organic nitrates, O_3, H_2O_2 and HCHO, for the final, net calculation for each grid cell and/or receptor, and as a function of the 16 generic land use types used in the TSD (see Table 1).

Table 1 provides the variables to be reported by all participants, the variable names as described in the AQMEII-4 TSDs, and a description of each variable. Note that equations (2) through (6) and related text describe these terms for the deposition framework of Wesely (1989). Further examples of the calculation of these terms are provided in the Tables and Figures that follow, as a guide to participants in AQMEII-4. Participants are asked to contribute a similar Figure and Table for their own resistance modules, as part of the deliverables for the intercomparison. Note that the *presence* of surface wetness or snow is tracked though other portions of the TSDs, but their effects should be incorporated into the effective conductances and component resistances (in other words, a separate component resistance or effective conductance for snow-covered or wet surfaces should *not* be reported).

Table 1. AQMEII-4 reported gas deposition variables.

Name as described here	AQMEII-4 Variable Name	Description
V_d	VD	Deposition velocity
r_a	RES-AERO	Aerodynamic resistance
r_c	RES-SURF	Bulk surface resistance
r_s	RES-STOM	Net stomatal resistance
r_m	RES-MESO	Net mesophyll resistance
r_c	RES-CUT	Net cuticle resistance
E_{STOM}	ECOND-ST	Effective conductance associated with deposition to plant stomata
E_{CUT}	ECOND-CUT	Effective conductance associated with deposition to plant cuticles
E_{SOIL}	ECOND-SOIL	Effective conductance associated with deposition to soil and un-vegetated surfaces
E_{LCAN}	ECOND-LCAN	Effective conductance associated with deposition to the lower canopy.
$r_{b,\ stom}$	RES-QLST	Quasi-laminar sublayer resistance associated with *stomatal pathway* (= r_b if this is pathway-independent for the deposition framework)
$r_{b,cut}$	RES-QLCT	Quasi-laminar sublayer resistance associated with cuticle pathway (= r_b if this is pathway-independent for the deposition framework)
$r_{b,soil}$	RES-QLSL	Quasi-laminar sublayer resistance associated with soil pathway (= r_b if this is pathway-independent for the deposition framework)
$r_{b,lcan}$	RES-QLLC	Quasi-laminar sublayer resistance associated with lower canopy pathway (= r_b if this is pathway-independent for the deposition framework)
r_{dc}	RES-CONV	Resistance associated with within-canopy convection.

Note that the net calculations (TSDs -012 to -122) should be carried out with the net values of the variables in the contributor's equivalent of equations (3) through (6) for individual land use types (these will be a post-processing calculation following output of the individual land use types).