Alaska Department of Environmental Conservation

Amendments to:
State Air Quality Control Plan

Volume III: Appendix III.K.2

IMPROVE Algorithms

Appendix to
Section III. K: Areawide Pollutant Control Program for Regional Haze

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IMPROVE Algorithms

Aerosol type equations

The IMPROVE network measures mass concentration data for many different aerosol species. Standard formulas are applied to derive additional visibility-related aerosol species. Typical Aerosol Type Equations are presented below [1]. Brackets indicate the mass concentration of the aerosol species or element. More detailed discussion on these aerosol type equations is found in Malm et al, 1994[2], the 2000 IMPROVE report[3] and the 1996 IMPROVE report[4].

SPECIES	Abbrev.	FORMULA	ASSUMPTIONS
Ammonium Sulfate	**SULFATE**	4.125[S]	All elemental S is from sulfate. All sulfate is from ammonium sulfate.
Ammonium Nitrate	**NITRATE**	1.29[NO_3]	Denuder efficiency is close to 100%. All nitrate is from ammonium nitrate.
Total Organic Carbon	**OC**	OC1+OC2+OC3+OC4+OP (see definitions below)	
Organic Mass by Carbon	**OMC**	1.4 * OC	Average organic molecule is 70% carbon.
Organic Carbon by Hydrogen	**OCH**	(11 * (H - 0.25 * S))	assumes all sulfur is ammonium sulfate and there is no hydrogen from nitrate. Organic mass is equal to 1.4*OCH
Light absorbing Carbon	**LAC**	EC1+EC2+EC3-OP	
fine soil	**SOIL**	2.2[Al]+2.49[Si]+1.63[Ca] +2.42[Fe]+1.94[Ti]	[Soil K]=0.6[Fe]. FeO and Fe_2O_3 are equally abundant. A factor of 1.16 is used for MgO, Na_2O, H_2O, CO_2.
reconstructed fine mass	**RCFM**	[SULFATE]+[NITRATE] +[LAC]+[OMC]+[SOIL]	Represents dry ambient fine aerosol mass for continental sites.
coarse mass	**CM**	[PM_{10}] - [$PM_{2.5}$]	Consists only of insoluble soil particles.

Light Extinction Equations (IMPROVE algorithms)

Chemically different aerosols affect visibility differently. Concentrations of aerosols (in μg/m3, from aerosol type equations) are converted to light extinction (visibility) by means of light extinction equations. There are currently two IMPROVE algorithms (or equations) used to convert measured aerosol concentrations to light extinction; these are referred to as the original (or old) and the revised (or new) IMPROVE algorithms. Both use mass concentration measurements and relative humidity estimates to calculate light extinction. Sulfate and nitrate are hygroscopic, taking on water and having greater light-scattering efficiencies under higher RH conditions. Relative humidity (RH) adjustment factors [f(RH)] are used to increase the Sulfate and nitrate particle's extinction efficiency with increasing RH. Further discussions of the two IMPROVE algorithms may be found in cited documents [4, 5].

Applications to Regional Haze Analysis

In Regional Haze analysis IMPROVE algorithms are used in describing Baseline visibility conditions, in defining Natural Visibility conditions to be attained by 2064, and in evaluating anticipated 2018 visibility improvement. For projected light extinctions (e.g. 2018 and 2064) the natural species concentration estimates used are from the NAPAP State of Science Report 24 by Trijonis[6].

Original IMPROVE Algorithm

The EPA adopted the original IMPROVE algorithm in their 2003 guidance document on *Tracking Progress Under the Regional Haze Rule* [7]. The equation for total light extinction combines extinctions by each chemical species, as measured by the IMPROVE aerosol monitors combined with the effects of Relative Humidity (RH), to estimate the scattering of light by fine and coarse particles.

The original IMPROVE algorithm converts particulate species concentrations to light extinction as follows, with the brackets indicating the species concentration and the prefix "b" denoting extinction. The factors 3, 4, 1, and 0.6 are the specific scattering efficiencies for each of the respective species. A sulfate particle, for instance, is three times more effective in scattering light than a particle of soil.

$$bSulfate = 3 \times f(RH) \times [Sulfate]$$
$$bNitrate = 3 \times f(RH) \times [Nitrate]$$
$$bEC = 10 \times [EC]$$
$$bOM = 4 \times [OMC]$$
$$bSoil = 1 \times [Soil]$$
$$bCM = 0.6 \times [CM]$$

The total light extinction (bext) is defined to be the sum of light extinction due to the six PM species listed above plus Rayleigh (blue sky) background (bRay) that is assumed to be 10 Mm-1:

$$bext = bRay + bSulfate + bNitrate + bEC + bOMC + bSoil + bCM$$

or

$$b_{ext} = 3f(RH)[sulfates] + 3f(RH)[nitrates] + 4[organics] + 10[elemental\ carbon] + 1[fine\ soil] + 0.6[coarse\ matter] + 10$$

Two related Measures used in Regional Haze Analysis are Visual Range (VR) and deciviews. The total light extinction (bext) in Mm^{-1} is related to VR in km using the following relationship: VR = 3912 / bext. The Regional Haze Rule requires that visibility be expressed in terms of a haze index in units of deciviews (dv), which is calculated as follows: HI = 10 ln(bext/10)

Revised IMPROVE Algorithm

In December 2005, the IMPROVE Steering Committee voted to adopt an alternative, revised algorithm for use by IMPROVE. The IMPROVE light extinction equation was analyzed, revised, and approved by the IMPROVE Steering Committee during 2005. In December 2005, the Steering Committee voted to adopt the alternative, revised algorithm for use by IMPROVE. The WRAP Technical Analysis Forum now recommends the use of the revised IMPROVE light extinction equation as developed and approved in 2005 by the IMPROVE Steering Committee to convert from mass concentration measurements to light extinction for visibility analysis and regional haze planning at each WRAP region Class I area. Detailed discussions of the revised equation and the reasons for changing the original are found in IMPROVE program publications[8,9,11].

The new equation splits ammonium sulfate, ammonium nitrate, and organic carbon compound concentrations into two size fractions: small and large. The equation for estimating the light extinction for the RHR is:

$$
\begin{aligned}
\text{bext} \approx\ & 2.2 \times \text{fs(RH)} \times [\text{small sulfate}] + 4.8 \times \text{fL(RH)} \times [\text{large sulfate}] \\
& + 2.4 \times \text{fs(RH)} \times [\text{small nitrate}] + 5.1 \times \text{fL(RH)} \times [\text{large nitrate}] \\
& + 2.8 \times [\text{small organic mass}] + 6.1 \times [\text{large organic mass}] \\
& + 10 \times [\text{elemental carbon}] \\
& + 1 \times [\text{fine soil}] \\
& + 1.7 \times \text{fss(RH)} \times [\text{sea salt}] \\
& + 0.6 \times [\text{coarse mass}] \\
& + \text{Rayleigh scattering (site-specific)} \\
& + 0.33 \times [\text{NO2 (ppb)}]
\end{aligned}
$$

Though not explicitly shown, the organic mass concentration used is 1.8 times the organic carbon mass concentration, (changed from 1.4 times carbon mass the original equation uses). New terms have also been added for sea salt and for absorption by NO2. The apportionment of the total concentration of sulfate compounds into the concentrations of small and large size fractions is accomplished using the following equations:

$$[\textit{large sulfate}] = [\text{total sulfate}] \times [\text{total sulfate}], \text{ for } [\text{total sulfate}] < 20\ \mu g/m3$$

$$[\textit{large sulfate}] = [\textit{total sulfate}], \textit{ for } [\textit{total sulfate}] \geq 20\ \mu g/m3$$

$$[\textit{small sulfate}] = [\textit{total sulfate}] - [\textit{large sulfate}]$$

The same equations are used to apportion total nitrate and total organic mass into small and large size fractions. Sea salt is calculated as 1.8 x [*chloride*], or 1.8 x [*chlorine*] if the chloride measurement is below detection limits, missing, or invalid. The new equation contains three distinct water growth terms, designated fS, fL, and fSS for the small and large sulfate and nitrate fractions, and for sea salt, respectively.

The new IMPROVE equation for estimating light extinction for the RHR contains five major revisions from the original equation[10]:

1) A sea salt term has been added. Sea salt is a particular concern for coastal locations where the sum of the major components of light extinction and mass has been deficient.
2) The assumed organic mass to organic carbon ratio has been changed from 1.4 to 1.8, to reflect more recent peer-reviewed literature on the subject.
3) The Rayleigh scattering factor has been changed from a network-wide constant to a site-specific value. This factor is based on the elevation and annual average temperature of individual monitoring sites.
4) A split component extinction efficiency model for sulfate, nitrate, and organic carbon components has been developed. The model includes new water growth terms for sulfate and nitrate to better estimate light extinction at the high and low extremes of the range of extinction.
5) An NO2 light absorption term has been added. This term can only be used at sites with available NO2 concentration data.

Use of the Revised IMPROVE Algorithm for Alaska's Regional Haze Analysis

Alaska has chosen to apply the revised IMPROVE algorithm for computing light extinctions. This follows the recommendation of the WRAP Technical Analysis Forum.

Several improvements in the revised algorithm affect Alaska specifically. The original IMPROVE equation tends to underestimate the highest extinction values and overestimate the lowest extinction values. Air at Alaska's Class 1 Areas is very clear, among the lowest extinction values nationwide, and impairment was overestimated by the original algorithm. In addition, three of Alaska's four Class 1 Areas are coastal, and visibility impairment from sea salt is extremely important at these sites. A sea salt term has been added to the revised algorithm.

Citations:

1 IMPROVE. available at: http://vista.cira.colostate.edu/improve/Tools/AerTypeEqs.htm

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3 James F. Sisler. 2000. Aerosol Mass Budgets and Spatial Distributions, Chapter 2 *in* Spatial and Seasonal Patterns and Temporal Variability of Haze and its Constituents in the United States: Report III, Principle Author: W. C. Malm.
Available at: http://vista.cira.colostate.edu/improve/Publications/Reports/2000/2000.htm

4 James F. Sisler. 1996. Optical and Aerosol Data, Chapter 2 *in* Spatial and Seasonal Patterns and Long Term Variability of the Composition of the Haze in the United States: An Analysis of Data from the IMPROVE Network, Report II. 1996, Principle Author: J. F. Sisler.
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5 Pitchford M. ; W. Malm; B. Schichtel; N. Kumar; D. Lowenthal; J. Hand. Revised algorithm for estimating light extinction from IMPROVE particle speciation data. J Air & Waste Manag Assoc 57 (11), pp. 1326-1336. 2007.

6 Trijonis, J.C., Malm, W.C., Pitchford, M.L., White, W.H., Charlson, R., and Husar, R. (1990) Visibility: Existing Conditions and Historical Conditions - Causes and Effects. *National Acid Precipitation Assessment Program State of the Science and Technology Volume III*, Report 24.

7 EPA Guidance for Tracking Progress Under the Regional Haze Rule. EPA-454/B-03-004 . September 2003. available at: http://www.epa.gov/ttn/oarpg/t1/memoranda/rh_tpurhr_gd.pdf).

8 http://vista.cira.colostate.edu/improve/Publications/NewsLetters/IMPNews4thQtr2005.pdf.

9 Applying_Monitoring_Metrics_for_Regional_Haze_Planning_%201_5_2007%20final%20draft.pdf available at http://vista.cira.colostate.edu/tss/Planning/InformationExchange.aspx

10 WRAP Technical Analysis Forum's Technical Recommendations on Monitoring Metrics for Regional Haze Planning 1/5/07 Final Draft.

11 http://vista.cira.colostate.edu/improve/Publications/GrayLit/019_RevisedIMPROVEeq/RevisedIMPROVEAlgorithm3.doc),

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