IV.

Use of Photochemical Reactivity as an Ozone Control Approach

A. Introduction

In this Chapter, we provide a description of how we propose to use the science of photochemical reactivity to control reactive organic compound (ROC) emissions from aerosol coatings. In Chapter II of this report, we provided background on the science of photochemical reactivity and the development of numerical scales that allow us to compare the differences in individual ROC reactivity. The potential of using reactivity as a ROC control approach has also been evaluated (Croes *et al*., 1992), and we believe the scientific foundation needed for using reactivity is well-established and readily available. In fact, hydrocarbon reactivity already serves as the basis for a portion of California's Low Emission Vehicle and Clean Fuels Regulation (LEV/CF) (ARB, 1990c). Research has also shown that reactivity-based control strategies have the potential to be a cost-effective approach to improve air quality (Russell *et al*., 1995; McBride *et al*., 1997).

The amendments proposed here would be the first reactivity-based regulation for non-mobile sources. To implement this reactivity-based regulation, we have developed a number of methods to apply the science of photochemical reactivity. These proposals are:

- Using the Maximum Incremental Reactivity (MIR) Scale
- Including Reactive Organic Compounds (ROC) that are Considered "Exempt" in Mass-Based Regulations
- Calculating Upper Limit MIR Values
- Calculating Group MIR Values for Hydrocarbon Solvent Mixtures
- Addressing Uncertainty in the Maximum Incremental Reactivity Scale
- Calculating "Equal Air Quality Benefit" Reactivity Limits

Our goal is to ensure that these amendments will achieve an ozone reduction equivalent to that which would be expected from implementation of the mass-based volatile organic compound (VOC) limits, while providing manufacturers with additional flexibility to achieve our air quality goals.

B. Program Elements

1. Using the Maximum Incremental Reactivity (MIR) Scale

As described in Chapter II, under a given environmental condition, organic compounds differ in their ozone forming abilities. In addition, individual chemicals are emitted into the atmosphere in the presence of other ROCs. These "background" organic compounds may have a modifying effect on a chemical's ozone forming potential (Bowman and Seinfield, 1994; Carter, 1994). In other words, a ROC not only contributes but also affects other compounds' abilities to react to form ozone. Therefore, to control emissions of ROCs, based on their potentials to form ozone, the air quality impact of an individual chemical as well as its effects on other ROCs needs to be assessed. To do this, in these amendments we are proposing to use the concept of MIR. The MIR is a numerical quantity that describes the change in peak ozone levels due to the addition of an organic compound under simulated atmospheric conditions. (Carter, 1994; 1998) (see also Chapter II).

Unlike the reactivity scales derived using the assumption that hydrocarbons occur singly in the atmosphere (see, for example, Bufalini et al., 1976), the MIR approach allows characterization of an individual organic compound's ability to form ozone, as well as its effect on other hydrocarbons (Carter, 1994; 2000). For this rulemaking, a list of over six hundred MIR values of ROC (in units of gram O_3 per gram organic compound) and representative chemical species (for example, branched C7 alkanes) has been compiled. These MIR values combined with emission data can be used to determine the ozone contribution of an individual chemical.

Under this proposal, manufacturers will need to assess the reactivity of their products by using the MIR scale. To do this, each ingredient in an aerosol coating formulation would be assigned its corresponding MIR value (non-ROCs are assigned MIR values of zero). The weight fraction of each ingredient is multiplied by the MIR value to get the "weighted reactivity" of an ingredient. The weighted reactivities of all ingredients are summed to get the product's weighted MIR (in grams ozone/gram product). The "product-weighted" MIR would then be compared to the reactivity limit to determine compliance. To comply, the product-weighted reactivity must be no more than the reactivity limit for the aerosol coating category. An example of how a product's weighted reactivity is calculated is provided in Appendix D.

2. Including "Exempt" Organic Compounds in Reactivity-based Regulations

The current Aerosol Coatings Regulation contains exemptions for "low reactive" VOCs, such as acetone, ethane, perchloroethylene, and parachlorobenzotrifluoride (PCBTF). This regulation essentially uses a reactivity scale of "zero" and "one" i.e. a compound is either exempt or assumed to have the same potential to form ozone as all other VOC compounds. This approach is consistent with that used by the United States Environmental Protection Agency (U.S. EPA) which classifies all VOCs as either “reactive” or “negligibly reactive” (Dimitriades, 1996). This “bright line” approach is practical for the implementation of mass-based regulations, but does not provide the level of detail to assess all ozone impacts of emitted VOCs.

Although the ability of organic compounds to induce ozone varies over several orders of magnitude (Carter, 2000), significant emissions of a “negligibly reactive” or “exempted VOC” under the current mass-based regulation may have a non-negligible air quality impact. An analysis of the 1997 Aerosol Coating Survey data indicate that the acetone (a “low reactive” exempt VOC) contained in aerosol coatings can change the reactivity of a product by 10 percent or more (ARB, 1998b). This provides evidence that in a reactivity program, the reactivities of low reactive VOCs should be considered with their respective smaller impacts on ozone formation. Hence, in this proposed regulation, all organic ingredients are included in evaluating the ozone forming potential of aerosol coating products.

3. Calculating Upper Limit MIR Values

The majority of ingredients used in aerosol coating products have MIR values available. However, there are several compounds currently used in aerosol coatings for which no published MIR value exists. To allow continued use of these ROCs a methodology for calculating upper limit MIRs was developed (Carter, 2000). This method for estimating the upper maximum incremental reactivity limit has been reviewed by the Reactivity Scientific Advisory Committee (RSAC) and is detailed in Appendix E of this report.

Briefly, the estimation procedure is based on deriving the upper limits of kinetic and mechanistic reactivities. Both of these factors play a critical role in determining the ozone impact of a compound in an air pollution episode (Carter and Atkinson, 1989). Kinetic reactivity is the fraction of a compound that reacts due to different atmospheric loss processes. Its upper limit, which has a maximum value of one, can be estimated using the rates of chemical reactions with different reactive species in the atmosphere (e.g. hydroxyl (OH) radicals). The number of ozone molecules formed for each molecule of ROC reacted is known as mechanistic reactivity. For determining the upper limit mechanistic reactivity of both photo- and non photo-reactive compounds, empirical relationships based on carbon number of a molecule or its hydroxyl radical reaction rate constant are established (Carter, 2000). The maximum incremental reactivity can be obtained by multiplying the upper limit estimates of kinetic reactivity and mechanistic reactivity.

4. Calculating Group MIR Values for Hydrocarbon Solvent Mixtures

Hydrocarbon solvents (HCS) are complex mixtures of organic compounds, which include alkanes, branched alkanes, cycloalkanes, and aromatics. Because different processes are used in their productions, these HCS have different compositions (CMA, 1997). Based on their chemical ingredients, HCS can be classified into aromatic and aliphatic solvents. Aromatic HCS are solvent mixtures containing approximately 100 percent of substituted monocyclic (i.e. single ring) and/or polycyclic (multiple rings) aromatic compounds. Aliphatic HCS are predominately saturated hydrocarbons, with maximum aromatic contents ranging from 2 to 22 percent by volume (see, for example, ASTM, 1995, CMA, 1997). Depending on their applications, different generic names are given to these aliphatic HCS, with "mineral spirit" being among the most commonly used name for those used in coatings industries (ASTM, 1995). Therefore, for evaluating the ozone formation potential of aerosol coating products, the ability to understand the reactivity of HCS is needed.

The reactivity of complex mixtures, such as HCS, can be calculated by combining each ingredient's MIR and its corresponding weight percentage (see for example, Chang and Rudy, 1990; McNair *et al.*, 1992). While computational methods exist for determining the MIR value of a chemical (see above), the detailed chemical speciation (i.e. ingredients) data needed for such a calculation may not be available for all HCS. To overcome this, if solvents can be assigned to a group, speciation profiles of selected or "typical" solvents may then be used for calculating a group reactivity. At present, however, there is no solvent categorization method available, although grouping criteria such as chemical abstract service (CAS) number, boiling ranges, and aromatic contents have been proposed.

To address the need, we have developed a categorization ("binning") methodology for hydrocarbon solvents. The procedure is detailed in the manuscript titled "Methods for Estimating Maximum Incremental Reactivity (MIR) of Hydrocarbon Solvents and Their Classification" (Kwok *et al.*, 2000) and is included as Appendix C of this report. Briefly, the hydrocarbon solvent classification scheme was developed by assuming that the overall HCS MIR can be estimated by summing the reactivity contribution from individual chemical classes. For hydrocarbon solvent mixtures composed of *n*-alkanes, branched alkanes, cycloalkanes, and mono-, di-, poly-substituted benzenes, the total MIR of a solvent mixture is then given by:

$$\begin{aligned} \text{HCS MIR} = {} & \text{Sum of \% Wt MIR of all straight-chain alkanes} \\ & + \text{Sum of \% Wt MIR of all branched alkanes} \\ & + \text{Sum of \% Wt MIR of all cycloalkanes} \\ & + \text{Sum of \% Wt MIR of all mono-substituted benzenes} \\ & + \text{Sum of \% Wt MIR of all di-substituted benzenes} \\ & + \text{Sum of \% Wt MIR of all poly-substituted benzenes} \end{aligned}$$

where % Wt = percent composition weighted.

To simplify the above equation, data suggest that for a given carbon number, the MIR values are relatively insensitive to the position of the substituent groups (see, for example, Carter, 2000). In addition, MIR values of C_{n-1}, C_n, and C_{n+1} homologs are similar (Carter, 2000), and hydrocarbon solvent mixtures have rather narrow carbon number distributions (see for example, Carter *et al*., 1997). Hence, the composition weighted (% Wt.) MIR of all compounds can be approximated by, for example, for branched (Br) alkanes:

Sum of % Wt MIR of all branched alkanes
= MIR of a Br-alkane
x total Wt % of Br-alkanes in the mixture

In other words, for a chemical class, the reactivity of all chemical species is similar, and a single species can be used to determine the reactivity contribution of the entire chemical class. Thus, the MIR of a complex HCS mixture can be calculated by using a simple n-alkane-branched-alkane-cycloalkane-aromatics mixture (i.e. surrogate mixture). Results from our analysis indicated that, in general, carbon number distribution of a HCS peaks at its average-boiling point, which is defined as the sum of initial boiling point (IBP) plus dry point (DP) divided by two. This relationship was used to identify the surrogate species of each chemical class. To validate these assumptions, solvent reactivities calculated using the surrogate mixture approach were tested against the HCS reactivity data reported by the solvent manufacturing industry. Based on this comparison, over 90 percent of the solvents tested have estimated and reported reactivity values that mostly differed by no more than a factor of 15 percent. This result shows that a surrogate mixture can be used for representing complex HCS for reactivity determinations.

In developing a way to group HCS of similar reactivity, it is important to ensure that the MIR value assigned for the group reliably reflects the reactivity of a particular HCS mixture within the group. Using the surrogate mixture procedure developed, calculations were performed to determine the effects of hydrocarbon composition (i.e. relative percentages of *n*-alkanes, branched alkanes, cycloalkanes, and aromatics) and carbon number (as a function of boiling point) on a mixture's MIR value. Our results indicate that, up to a certain temperature range, solvent composition has only a minor effect on the mixture MIR value. Using a surrogate mixture MIR's coefficients of variation of 15 percent as a grouping criterion, we have developed four HCS reactivity groups over the average boiling point of 80-580 ^{o}F. This temperature range is consistent with the existing HCS data. Within each group, five different sub-groups are defined according to their dominant chemical ingredients. The aromatic content of these solvents is classified according to the American Society of Testing and Materials method (ASTM, 1995).

To assist aerosol coating formulators with applying this HCS classification scheme, typical solvent sales specification data such as mid-boiling range, percent total alkanes and isoalkanes, cyclolkanes and aromatics are used as categorization criteria. Table IV-1 lists all twenty aliphatic hydrocarbon solvent bins and their corresponding group MIR values. In most cases (~70 percent), the assigned MIR is approximately ± 15 percent of the reported values, and only a few (~ 7 percent) have a discrepancy between the assigned and reported values greater than 30 percent.

TABLE IV-1
PROPOSED DRAFT APPROACH FOR ASSIGNING MIR VALUES TO ALIPHATIC HYDROCARBON SOLVENTS

Average BP (oF)	CRITERIA	MIR (g O3/g Organics)	BIN NO.
80-205	ALKANES (< 2% AROMATICS)	2.08	1
	N- & ISO-ALKANES (≥ 90% & < 2% AROMATICS)	1.59	2
	CYCLO-ALKANES (≥ 90% & < 2% AROMATICS)	2.52	3
	ALKANES (2 to < 8% AROMATICS)	2.24	4
	ALKANES (8 to 22% AROMATICS)	2.56	5
> 205-340	ALKANES (< 2% AROMATICS)	1.41	6
	N- & ISO-ALKANES (≥ 90% & < 2% AROMATICS)	1.17	7
	CYCLO-ALKANES (≥ 90% & < 2% AROMATICS)	1.65	8
	ALKANES (2 to < 8% AROMATICS)	1.62	9
	ALKANES (8 to 22% AROMATICS)	2.03	10
> 340-460	ALKANES (< 2% AROMATICS)	0.91	11
	N- & ISO-ALKANES (≥ 90% & < 2% AROMATICS)	0.81	12
	CYCLO-ALKANES (≥ 90% & < 2% AROMATICS)	1.01	13
	ALKANES (2 to < 8% AROMATICS)	1.21	14
	ALKANES (8 to 22% AROMATICS)	1.82	15
> 460-580	ALKANES (< 2% AROMATICS)	0.57	16
	N- & ISO-ALKANES (≥ 90% & < 2% AROMATICS)	0.51	17
	CYCLO-ALKANES (≥ 90% & < 2% AROMATICS)	0.63	18
	ALKANES (2 to < 8% AROMATICS)	0.88	19
	ALKANES (8 to 22% AROMATICS)	1.49	20

TABLE IV-2
PROPOSED DRAFT APPROACH FOR ASSIGNING MIR VALUES TO AROMATIC HYDROCARBON SOLVENTS

Boiling Range (oF)	CRITERIA	MIR (g O3/g Organics)	BIN NO.
280-290	100% AROMATICS	7.37	21
320-350	100% AROMATICS	7.51	22
355-420	100% AROMATICS	8.07	23
450-535	100% AROMATICS	5.00	24

For aromatic hydrocarbon solvents, the speciation data are scarce, and the surrogate mixture approach was not used for determining the solvent reactivity. Hence, the aromatic HCS classification scheme was constructed based on the boiling range and is presented in Table IV-2 (Bin 21-24).

5. Addressing Uncertainty in the Maximum Incremental Reactivity Scale

As described in Chapter II, there are uncertainties associated with reactivity scales such as the MIR. Therefore, to apply reactivity as a control approach, we believe that most of the ROCs used in the category proposed for regulation need to consist of well-characterized compounds (i.e. with “certain” MIR values). In addition, a method to account for MIR value uncertainty is needed. In the aerosol coatings category, over 80 percent of ROCs used are well-studied and an additional 17 percent of the inventory (i.e. hydrocarbon solvents) would need only a minor adjustment for uncertainty. In other words, over 95 percent of the ROCs used in aerosol coatings are fairly well-characterized in terms of their reactivity. Nevertheless, to ensure that the total air quality benefit is achieved, we believe uncertainty factors should still be applied when appropriate. Below we describe our proposal for using uncertainty “factors” in the proposed amendments.

Based on the analysis in Chapter II, we concluded that for regulatory applications uncertainty adjustments should be tied to the individual compound. Therefore, following the recommendation of Dr. Carter and using his uncertainty “bin” assignments, we are proposing to apply uncertainty factors to individual compounds. For our proposed amendments to the Aerosol Coatings Regulation, we propose to apply an uncertainty factor of 1.0 to compounds classified within uncertainty bins one and two; a factor of 1.25 to compounds in bin three; a factor of 1.5 to compounds in bin four; and a factor of 2.0 for compounds in bins five and six.

Organic compounds in uncertainty bins one and two are compounds which have been studied extensively (in most cases) in the laboratory, and their ozone forming ability can be reasonably described by the chemical mechanism developed. Hence, no adjustment is recommended for bin one and two chemicals. As mentioned previously, over 80 percent (on a weight basis) of ROCs used in aerosol coatings would fall into bins one and two. Bin three chemicals, constitute two percent of compounds used in aerosol coatings (ARB, 1998b). These chemicals, in general, have lesser amounts of experimental data available, and a slight change to the MIR value could occur when the chemical mechanism is refined in the future. Because of this, an adjustment factor of 1.25 is proposed.

Bin four chemicals, include “generic” species representing the reactivity of a group of chemicals. The higher adjustment factor recommended for bin four chemicals (i.e. 1.5 compared to 1.25 for bin three) is consistent with the lack of experimental data for this group. However, less than one percent of compounds reported in the 1997 survey would fall into bin four (ARB, 1998b). Although some chemicals in bins five and six have been tested under laboratory conditions, the modeling results are not conclusive.

Hence, an uncertainty factor of 2.0 is proposed. Less than one percent of aerosol coating ROCs reported in the survey fall into bins five and six (ARB, 1998b).

For hydrocarbon solvent MIRs shown in Table IV-1 and II, an uncertainty factor of 1.15 is proposed. By proposing this factor, we are assuming that the HCS table MIR values provide a reliable description of the "true" solvent's reactivity. The adjustment factor proposed is to account for the need to "bin" HCS into groups as described earlier. For estimated MIR values (i.e. upper limit MIRs), no adjustment factor is proposed as the method used infers the highest reactivity of the chemical.

ARB staff recognizes that for compounds with uncertain MIR values it is likely that, upon further study, the MIR value for an individual compound may increase or may decrease. However, to ensure the air quality benefit, staff is proposing to increase the reported MIR value by multiplying it by the uncertainty factor. This conservative approach preserves the air quality benefit.

Uncertainty factors can be applied in two ways. MIR values can be adjusted when calculating the reactivity limit or can be adjusted when manufacturers determine the reactivity of their products. Either approach should preserve the air quality benefit. Both proposals were presented to the aerosol coatings industry and their preference was to apply uncertainty factors to calculation of the reactivity limit. In this way manufacturers can determine the reactivity of their products by using the MIR values as they appear in the Tables of MIR values.

6. Calculating "Equal Air Quality Benefit" Reactivity Limits

In this rulemaking, we are proposing to replace the January 1, 2002, mass-based aerosol coating VOC limits with equivalent reactivity limits. For aerosol coatings, because a mass-based reduction has already been claimed we need to ensure this commitment will be met. Hence, a common basis is needed to compare the air quality benefit from mass-based versus reactivity-based control, which in this case, is the amount of ozone reduction to be achieved. Based on the premise of providing an equal air quality benefit, the proposed methodology is designed to develop a reactivity limit that will match the amount of ozone reductions associated with implementation of the mass-based standards.

The calculation involves two simple steps. Step one is to determine the amount of ozone reduction that would be achieved from the mass-based VOC reduction. The reactivity limit is then set using an iterative process until the target ozone reduction is matched. The sales and VOC content data relied upon for this rulemaking are obtained from the Air Resources Board 1997 Aerosol Coating Product Survey (ARB, 1998b). These procedures are detailed below.

To calculate the ozone reduction achieved by the mass-based limits, we assumed that the average reactivity of all VOCs used in a particular aerosol coating product category could be represented by an overall sales-weighted average maximum incremental reactivity ($\text{SWA-MIR}_{\text{VOC}}$) (in units of g O_3/g organics). In other words, this metric describes the ozone formation potential contributed by the VOCs. This can be expressed in the following equation:

$$\text{SWA-MIR}_{\text{VOC}} = \text{SWA-MIR}_{\text{prod}} / \text{SWA-VOC}, \qquad (1)$$

Where:

$\text{SWA-MIR}_{\text{prod}}$ = Sales-weighted average product MIR

= Summation of the products’ individual reactivities multiplied by their individual sales divided by the summation of the sales in the product category

SWA-VOC = Sales-weighted average VOC

= Summation of the products’ individual VOC contents multiplied by their individual sales divided by the summation of the sales in the product category.

Under the mass-based regulation, ozone reductions would only be achieved from the reduction of non-exempted VOC emissions. The total amount of ozone reduction from the mass-based control then, would be equal to the $\text{SWA-MIR}_{\text{VOC}}$ multiplied by the total amount of non-exempted VOCs ($\text{VOC}_{\text{non-exempt}}$) exceeding the particular VOC limit ($\text{VOC}_{\text{limit}}$).

Ozone Reduction from an Aerosol Coatings Product Category

$$= \text{SWA-MIR}_{\text{VOC}} \times (\text{VOC}_{\text{non-exempt}} - \text{VOC}_{\text{limit}}) \qquad (2)$$

In the calculation described above, the MIR values of individual ROCs have been adjusted for uncertainty based on our proposal described earlier in this Chapter. We believe that the application of adjustment factors in determining the target ozone reduction is a necessary conservative approach to ensure that the full ozone reduction is achieved.

Once the target ozone reduction is determined, the reactivity limit is calculated using the following procedures. The existing product reactivity (PWMIR) (in units of g O_3/g product) is calculated using its ingredient information and the unadjusted MIR values of all ingredients (non-ROC s are assigned MIR values of zero). A trial or arbitrary limit is then set. For those products with reactivity greater than the trial limit, the amount of ozone reduced due to the "reactivity reduction" is calculated by the following equation:

$$\text{Ozone Reduction} = (\text{PWMIR} - \text{"Limit"}) \times \text{Sales} \qquad (3)$$

This step is then repeated for all "non-complying" products, and the expected ozone reduction from the trial limit applied to each product are summed. The total ozone reduction is calculated for each trial limit (i.e. iteration) and is repeated until it equals the mass-based target ozone reduction. The VOC reduction, adjusted SWA-MIR_{VOC}, and target ozone reduction (i.e. adjusted equivalent ozone reduction) for all categories are listed in Chapter IX, Tables IX-1 through IX-16.

The advantage of this "trial-and-error" method is that it allows products with more reactive organic compounds to be "selectively" controlled. This is because the product's reactivity is evaluated based on its entire formulation. This is believed to be a more appropriate method for evaluating air quality benefits using ROC substitution (Carter, 1999). In addition, using this method, no assumptions are made regarding future product ingredients and ROC contents in this computational exercise. Therefore, the results obtained will reliably reflect the air quality benefit expected from the reactivity-based regulation.

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