

APPENDIX M

Chemical Mechanism and Process Analysis Details

Chemical Mechanism and Process Analysis Details

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Table M-1. Gas-Phase Chemical Species for RADM2 Mechanism (plus CIS_1)

CHEMICAL SPECIES IN RADM2:

Stable Inorganic Compounds

<u>Nitrogen</u>	<u>Variable Name</u>	<u>Description</u>
NO ₂	NO2	Nitrogen dioxide
NO	NO	Nitric oxide
HONO	HONO	Nitrous acid
NO ₃	NO3	Nitrogen trioxide
N ₂ O ₅	N2O5	Nitrogen pentoxide
HNO ₄	HNO4	Pernitric acid
HNO ₃	HNO3	Nitric acid

Oxidants

O ₃	O3	Ozone
H ₂ O ₂	H2O2	Hydrogen peroxide

Sulfur

SO ₂	SO2	Sulfur dioxide
SULF	SULF	Sulfuric acid

Carbon Oxides

CO	CO	Carbon monoxide
CO ₂	CO2	Carbon dioxide (product only)
H ₂	H2	Hydrogen (product only)

Inorganic Short-Lived Intermediates

Atomic Species

O ³ P	O3P	Ground state oxygen atom
O ¹ D	O1D	Excited state oxygen atom

Odd Hydrogen

HO	HO	Hydroxy radical
HO ₂	HO2	Hydroperoxy radical

Abundant Stable Species

O ₂	O2	Oxygen
N ₂	N2	Nitrogen
H ₂ O	H2O	Water

Stable Organic Compounds

Alkanes

CH ₄	CH4	Methane
ETH	ETH	Ethane

HC3	HC3	Alkanes with HO rate constant (298, 1 atm) between 2.7×10^{-13} and 3.4×10^{-12}
HC5	HC5	Alkanes with HO rate constant (298, 1 atm) between 3.4×10^{-12} and 6.8×10^{-12}
HC8	HC8	Alkanes with HO rate constant (298, 1 atm) greater than 6.8×10^{-12}
<u>Alkenes</u>		
OL2	OL2	Ethene
OLT	OLT	Terminal alkenes
OLI	OLI	Internal alkenes
ISO	ISO	Isoprene
TOL	TOL	Toluene and less reactive aromatics
CSL	CSL	Cresol and other hydroxy substituted aromatics
XYL	XYL	Xylene and more reactive aromatics
<u>Carbonyls</u>		
HCHO	HCHO	Formaldehyde
ALD	ALD	Acetaldehyde and higher aldehydes
KET	KET	Ketones
GLY	GLY	Glyoxal
MGLY	MGLY	Methylglyoxal
DCB	DCB	Unsaturated Dicarbonyl
<u>Organic Nitrogen</u>		
PAN	PAN	Peroxyacetyl nitrate and higher PANs
TPAN	TPAN	$\text{H}(\text{CO})\text{CH}=\text{CHCO}_3\text{NO}_2$
ONIT	ONIT	Organic nitrate
<u>Organic Peroxides</u>		
OP1	OP1	Methyl hydrogen peroxide
OP2	OP2	Higher organic peroxides
PAA	PAA	Peroxyacetic acid
<u>Organic Acids</u>		
ORA1	ORA1	Formic acid
ORA2	ORA2	Acetic acid and higher acids

Organic Short-Lived Intermediates

Peroxy Radicals from Alkanes

MO ₂	MO2	Methyl peroxy radical
ETHP	ETHP	Peroxy radical formed from alkane, ETH
HC3P	HC3P	Peroxy radical formed from alkane, HC3
HC5P	HC5P	Peroxy radical formed from alkane, HC5
HC8P	HC8P	Peroxy radical formed from alkane, HC8

Peroxy Radicals from Alkenes

OL2P	OL2P	Peroxy radical formed from alkene, OL2
OLTP	OLTP	Peroxy radical formed from alkene, OLT
OLIP	OLIP	Peroxy radical formed from alkene, OLIP
<u>Peroxy Radicals from Aromatics</u>		
TOLP	TOLP	Peroxy radical formed from aromatic, TOL
XYLP	XYLP	Peroxy radical formed from aromatic, XYL
<u>Peroxy Radicals with Carbonyl Groups</u>		
ACO ₃	ACO3	Acetylperoxy Radical
KETP	KETP	Peroxy radical formed from ketone, KET
TCO ₃	TCO3	H(CO)CH=CHCO ₃
<u>Peroxy Radicals Involving Nitrogen</u>		
OLN	OLN	NO ₃ -alkene adduct
XNO ₂	XNO2	Accounts for additional organic nitrate
XO ₂	XO2	Accounts for additional NO to NO ₂ conversions affected by the lumped species

Additional species in RADM2_CIS1:

Peroxy Radicals from isoprene reactions:

ISO_RO2
ISON_RO2
IP_RO2

Lumped products from isoprene reactions:

ISOPROD

Species added to RADM2 for aerosols:

Counter species to track reaction rates:

SULAER
HC8AER
OLIAER
TOLAER
XYLAER
CSLAER
TERPAER

Monoterpenes:

TERP

Table M-2. Gas-Phase Chemical Species for the CB-IV Mechanism (plus AQ)

Chemical Species in the CBM-IV:

Stable Inorganic Compounds

<u>Nitrogen</u>	<u>Variable</u>	<u>Description</u>
NO	NO	Nitric oxide
NO ₂	NO2	Nitrogen dioxide
NO ₃	NO3	Nitrogen trioxide
N ₂ O ₅	N2O5	Dinitrogen pentoxide
HONO	HONO	Nitrous acid
HNO ₃	HNO3	Nitric acid
PNA	PNA	Peroxynitric acid (HO ₂ NO ₂)

Inorganic Short-Lived Intermediate

Atomic Species

O1D	O1D	Oxygen atom (singlet)
O	O	Oxygen atom (triplet)

Odd Hydrogen

OH	OH	Hydroxyl radical
HO ₂	HO2	Hydroperoxy radical

Abundant Stable Species

H ₂ O	H2O	Water
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Oxidants

O ₃	O3	Ozone
H ₂ O ₂	H2O2	Hydrogen peroxide

Carbon Oxides

CO	CO	Carbon monoxide
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Stable Organic Compounds

FORM	FORM	Formaldehyde (CH ₂ =O)
ALD ₂	ALD2	High molecular wt. aldehydes (RCHO, R>H)
C ₂ O ₃	C2O3	Peroxyacetyl radical (CH ₃ C(O)OO)
PAN	PAN	Peroxyacetyl nitrate (CH ₃ C(O)OONO ₂)
PAR	PAR	Paraffin carbon bond (C-C)
ROR	ROR	Secondary organic oxy radical
OLE	OLE	Olefinic carbon bond (C=C)
ETH	ETH	Ethene (CH ₂ =CH ₂)
TOL	TOL	Toluene (C ₆ H ₅ -CH ₃)
CRES	CRES	Cresol and higher molecular weight phenols

Stable Organic Compounds (continued)

TO ₂	TO2	Toluene-hydroxyl radical adduct
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CRO	CRO	Methylphenoxy radical
OPEN	OPEN	High molecular weight aromatic oxidation ring fragment
XYL	XYL	Xylene ($C_6H_4-(CH_3)_2$)
MGLY	MGLY	Methylglyoxal ($CH_3C(O)C(O)H$)
ISOP	ISOP	Isoprene
XO_2	XO_2	NO-to- NO_2 operation
XO_2N	XO_2N	NO-to-nitrate operation

Species added to CB4 for aerosols:

Counter species to track reaction rates:

SULAER
 TOLAER
 XYLAER
 CSLAER
 TERPAER

Monoterpenes:

TERP

Species added to CB4 for aqueous chemistry:

Formic Acid	FACD
Acetic and higher Acids	AACD
Peroxy Acetic Acid	PACD
Upper limit of methylhydroperoxide	UMHP

Table M-3. Aerosol Species and Molecular Weights

<u>Description</u>	<u>Species Name</u>	<u>Molecular weight</u>
Accumulation mode sulfate aerosol	ASO4J	96.0
Aitken mode sulfate aerosol	ASO4I	96.0
Accumulation mode ammonium aerosol	ANH4J	18.0
Aitken mode ammonium aerosol	ANH4I	18.0
Accumulation mode nitrate aerosol	ANO3J	62.0
Aitken mode nitrate aerosol	ANO3I	62.0
Accumulation mode anthropogenic secondary organic aerosol	AORGA	120.0
Aitken mode anthropogenic secondary organic aerosol	AORGAI	120.0
Accumulation mode primary organic aerosol	AORGPAJ	120.0
Aitken mode primary organic aerosol	AORGPAI	120.0
Accumulation mode biogenic secondary organic aerosol	AORGB	120.0
Aitken mode biogenic secondary organic aerosol	AORGBI	120.0
Accumulation mode elemental carbon	AECJ	12.0
Aitken mode elemental carbon	AECI	12.0
Accumulation mode unspecified anthropogenic aerosol	A25J	200.0
Aitken mode unspecified anthropogenic aerosol	A25I	200.0
Coarse mode unspecified anthropogenic aerosol	ACORS	100.0
Coarse mode marine aerosol	ASEAS	58.0
Coarse mode soil-derived aerosol	ASOIL	100.0
Aitken mode number concentration	NUMATKN	1.0
Accumulation mode number concentration	NUMACC	1.0
Coarse mode number concentration	NUMCOR	1.0
Accumulation mode water concentration	AH2O	18.0
Aitken mode water concentration	AH2OI	18.0

Table M-4. Names for RADM2 and CB-IV Emission Species

<u>Description</u>	<u>RADM2 Emission Name</u>	<u>CB4 Emission Name</u>
Nitrogen oxide	NO	NO
Nitrogen dioxide	NO2	NO2
Carbon monoxide	CO	CO
Sulfur dioxide	SO2	SO2
Sulfuric acid	SULF	SULF
Ammonia	NH3	NH3
Particulates < 2.5um	PM2_5	PM2_5
Particulates < 10um	PM10	PM10
Ethene	OL2	ETH
Formaldehyde	HCHO	FORM
Acetaldehyde	ALD	ALD2
Isoprene	ISO	ISOP
Toluene	TOL	TOL
Xylene	XYL	XYL
Biogenic terpenes	TERPB	TERPB
Ethane	ETH	
Slow reacting alkanes HC3		
Medium reacting alkanes	HC5	
Fast reacting alkanes	HC8	
Terminal alkenes	OLT	
Internal alkenes	OLI	
Cresol	CSL	
Ketones	KET	
Acetic acid	ORA2	
Paraffins		PAR
Olefins		OLE

Note: Missing species name indicates species not defined for that mechanism.

Table M-5. Deposition Velocity Surrogate Names

<u>Description</u>	<u>CMAQ Surrogate Name</u>
<u>Gas-phase species:</u>	
Nitrogen oxide	VD_NO
Nitrogen dioxide	VD_NO2
Ozone	VD_O3
Nitric acid	VD_HNO3
Hydrogen peroxide	VD_H2O2
Sulfur dioxide	VD_SO2
Sulfuric acid	VD_SULF
Formaldehyde	VD_HCHO
Acetaldehyde	VD_ALD
Peroxyacetic acid	VD_PAA
Organic peroxides	VD_OP
Organic acids	VD_ORA
<u>Aerosol species:</u>	
Accumulation mode mass	VMASSJ
Aitken mode mass	VMASSI
Coarse mode mass	VMASSC
Accumulation mode number	VNUMACC
Aitken mode number	VNUMATKN
Coarse mode number	VNUMCOR
<u>Non-reactive species:</u>	
Ammonia	VD_NH3

Table M-6. Surrogate Names for Gas/Aerosol/Aqueous Chemistry/Non-Reactive/Tracer Links

<u>Description</u>	<u>Surrogate Name</u>
<u>Gas to Aerosol links (G2AE):</u>	
Nitric acid	HNO3
Sulfuric acid	SULF
Terpenes	TERPSP
Alkane reaction rate counter species	ALKRXN
Olefin reaction rate counter species	OLIRXN
Toluene reaction rate counter species	TOLRXN
Xylene reaction rate counter species	XYLRXN
Cresol reaction rate counter species	CSLRXN
Terpene reaction rate counter species	TERPRXN
<u>Gas to Aqueous Chemistry links (G2AQ):</u>	
Nitric acid	HNO3
Sulfuric acid	H2SO4
Sulfur dioxide	SO2
Nitrogen pentoxide	N2O5
Hydrogen peroxide	H2O2
Ozone	O3
Formic acid	FOA
Peroxy acetic acid	PAA
Methyl hydrogen peroxide	MHP
<u>Aerosol to Aqueous Chemistry links (A2AQ):</u>	
Aitken mode sulfate aerosol	SO4_AITKEN
Accumulation mode sulfate aerosol	SO4_ACCUM
Aitken mode ammonium aerosol	NH4_AITKEN
Accumulation mode ammonium aerosol	NH4_ACCUM
Aitken mode nitrate aerosol	NO3_AITKEN
Accumulation mode nitrate aerosol	NO3_ACCUM
Coarse mode nitrate aerosol	NO3_COARSE
Aitken mode organic aerosol	ORG_AITKEN
Accumulation mode organic aerosol	ORG_ACCUM
Aitken mode primary aerosol	PRI_AITKEN
Accumulation mode primary aerosol	PRI_ACCUM
Coarse mode primary aerosol	PRI_COARSE
Calcium carbonate	CACO3
Magnesium carbonate	MGCO3

Table M-6. Surrogate Names for Gas/Aerosol/Aqueous Chemistry/Non-Reactive/Tracer Links (continued)

<u>Description</u>	<u>Surrogate Name</u>
Sodium chloride	NACL
Iron	A3FE
Manganese	B2MN
Potassium chloride	KCL
Aitken mode number concentration	NUM_AITKEN
Accumulation mode number concentration	NUM_ACCUM
Coarse mode number concentration	NUM_COARSE

Non-reactive to aerosol links (N2AE):

Ammonia	NH3
---------	-----

Non-reactive to Aqueous chemistry links (N2AQ):

Ammonia	NH3
Carbon dioxide	CO2

Table M-7. Surrogate Names for Cloud Scavenging (AQ)

<u>Chemical Compound</u>	<u>Surrogate Name</u>
<u>Gas-phase species:</u>	
Ozone	O3
Hydroxy radical	HO2
Hydrogen peroxide	H2O2
Nitric oxide	NO
Nitrogen dioxide	NO2
Nitrate radical	NO3
Nitrogen pentoxide	N2O5
Nitrous acid	HNO2
Nitric acid	HNO3
Pernitric acid	HNO4
Sulfur dioxide	SO2
Sulfuric acid	H2SO4
Methane	METHANE
Ethane	ETHANE
Propane	PROPANE
Butane	BUTANE
Pentane	PENTANE
Hexane	HEXANE
Octane	OCTANE
Nonage	NONAGE
Decade	DECADE
Ethene	ETHENE
Propene	PROPENE
Isoprene	ISOPRENE
Acetylene	ACETYLENE
Benzene	BENZENE
Toluene	TOLUENE
O-xylene	O-XYLENE
Methanol	METHANOL
Ethanol	ETHANOL
2-cresol	2-CRESOL
4-cresol	4-CRESOL
Methyl hydrogen peroxide	METHYLHYDROPEROX
Formaldehyde	FORMALDEHYDE
Acetaldehyde	ACETALDEHYDE
Generic aldehyde	GENERIC_ALDEHYDE

Table M-7. Surrogate Names for Cloud Scavenging (AQ) (continued)

Glyoxal	GLYOXAL
Acetone	ACETONE
Formic acid	FORMIC_ACID
Acetic acid	ACETIC_ACID
Methyl glyoxal	METHYL_GLYOXAL
Carbon monoxide	CO
Peroxyacetyl nitrate and higher PANs	PAN
Peroxyacetyl nitrate compound produced from methacrolein	MPAN
Hydroxy radical	OH
Methyl-peroxy radical	METHYLPEROXY_RAD
Peroxy acetic acid	PEROXYACETIC_ACI
<u>Aerosol species:</u>	
Accumulation mode sulfate aerosol	SO4_ACCUM
Aitken mode sulfate aerosol	SO4_AITKEN
Accumulation mode ammonium aerosol	NH4_ACCUM
Aitken mode ammonium aerosol	NH4_AITKEN
Accumulation mode nitrate aerosol	NO3_ACCUM
Aitken mode nitrate aerosol	NO3_AITKEN
Accumulation mode anthropogenic secondary organic aerosol	ORGA_ACCUM
Aitken mode anthropogenic secondary organic aerosol	ORGA_AITKEN
Accumulation mode primary organic aerosol	ORGPA_ACCUM
Aitken mode primary organic aerosol	ORGPA_AITKEN
Accumulation mode biogenic secondary organic aerosol	ORGB_ACCUM
Aitken mode biogenic secondary organic aerosol	ORGB_AITKEN
Accumulation mode elemental carbon	EC_ACCUM
Aitken mode elemental carbon	EC_AITKEN
Accumulation mode unspecified anthropogenic aerosol	A25_ACCUM
Aitken mode unspecified anthropogenic aerosol	A25_AITKEN
Coarse mode unspecified anthropogenic aerosol	CORS
Coarse mode marine aerosol	SEAS
Coarse mode soil-derived aerosol	SOIL

Table M-7. Surrogate Names for Cloud Scavenging (AQ) (continued)

Aitken mode number concentration	NUM_AITKEN
Accumulation mode number concentration	NUM_ACCUM
Coarse mode number concentration	NUM_COARSE
Accumulation mode water concentration	H2O_ACCUM
Aitken mode water concentration	H2O_AITKEN

Non-reactive species:

Ammonia	NH3
Carbon dioxide	CO2

Gas-Phase Chemical Reactions Input Format

Introduction. The Models-3/CMAQ system employs a generalized chemical mechanism processor (MP) for gas-phase chemical mechanisms. The generalized processor greatly simplifies the task of altering chemical mechanisms and provides the capability of easily using different mechanisms in the CMAQ system. This appendix describes the format that must be used for entering a gas-phase chemical mechanism in the CMAQ system. As described in Section 11.4.1, the mechanism can be entered directly in the Models-3 framework or can be imported into the system via an ASCII text file that contains the reaction data. Since gas-phase chemical mechanisms are usually lengthy, the latter approach is recommended. The ASCII file can be created with any editor or word processor that generates a standard ASCII file.

The gas-phase mechanism data are formatted according to a simple set of rules and a free-form format that are similar to the approaches used by Jeffries et al. (1990) and Gery and Crouse (1990). For reference, example listings of two chemical mechanism input files are included at the end of this appendix. The mechanism input data consist of four major parts: an optional mechanism name, a Reactions keyword that can be used to specify the units of the rate coefficients, a series of reaction and rate constant lines, and an end of reactions list keyword. Each of these will be discussed separately below. The discussion begins first, however, with a description of some general rules for entering the mechanism data.

General rules. The free-form format generally ignores white spaces and allows line wrap around (i.e., entries can be continued on a subsequent line after a hard return). The free-form format also allows embedded comments and makes use of special symbols to indicate the type of input data. Special rules for naming species, entering labels, and specifying numerical values, such as stoichiometric coefficients and rate constant parameters, are also used. Each is discussed below.

Comments. All lines that have an exclamation point in column 1 are treated as comment lines and are ignored by the MP. Any text enclosed in braces or parentheses is also treated as comment and ignored by the MP.

Species names. The MP recognizes two types of species names: predefined and user-defined. The predefined names include M (any molecule in the atmosphere), O₂ (oxygen), N₂ (nitrogen), and H₂O (water vapor). These particular species can be referenced anywhere in the mechanism using the short names but should not be used to represent any other species in the mechanism. The following special rules have also been established for user-defined species names.

- a) The input names must not contain any blanks and can be up to 81 characters long, but only the first 16 characters are significant.
- b) The name must begin with an alphabetic character, but may contain any alphanumeric character (i.e., "A-Z," "a-z," and "0-9") or the characters ":" and "_" after the first position.
- c) The name is case sensitive. Thus, NO₂ and no₂ would represent two different species.
- d) A name can have embedded comments but cannot span two lines.

Label names. Special rules also apply to label names that are used in the chemical reaction definitions.

- a) A label is defined as any string starting with the character "<" and ending with ">".
- b) A label can be up to 81 characters long, but only the first 16 non-blank characters are used.
- c) A label may contain any character except a single comment or a label delimiter. Embedded blanks in the label name are discarded.
- d) A label can span lines and contain embedded comments.

Numbers. Numerical inputs can be either integer (e.g., 5), floating point (e.g., 5.0), or exponential (e.g., 5.0E+00). With the exponential format, the "E" may be either upper or lowercase; a positive exponent will be assumed if the sign of the exponent is missing.

Mechanism Name. The mechanism name is an optional input. If it is included, it must be the first non-comment entry in the mechanism. The name entered in the input file is *not* the name that will be used in the Models-3 framework, however. The name assigned here will be output in a comment line in the mechanism include files that are generated by the MP, but it is not used by any CMAQ processor or model. Rules for the mechanism name are the same as those for species names, except that only the first eight characters are used. Although no delimiter is required at the end of the name, a "hard return" after the entry is suggested for clarity in reading the input file.

Reaction Keyword. The list of reactions must be preceded by the symbolic keyword REACTIONS, but only the first four characters (i.e., REAC) are actually required. If no mechanism name is supplied, it would be the first non-comment entry. The reaction key word is followed by a units keyword, enclosed in brackets, to indicate the units of the input rate constants that are to follow. The units options are "PP" and "CM," which stand for ppm-min units and molecule-cc-sec units, respectively. (Note that longer entries could be used, but only the first two characters are significant. Also, the first two characters can either be upper or lowercase provided they are both of the same case). Finally, the units option must be followed by an equal sign (=). A delimiter is not required after the equal sign, but a "hard return" after the entry is suggested for clarity in reading the input file. Examples of valid inputs include the following:

```
REAC[PP]=  
REACTIONS[CM]=  
REACTIONS[ppm]=  
REAC[cms]=
```

Reaction Definitions. The reaction keyword is followed by a cluster of "reaction lines." The reaction lines consist of the following: 1) an optional label, 2) up to 3 reactants 3) an equal sign (=) to separate reactants from products, 4) up to 12 products with optional numerical coefficients, 5) a reaction rate constant in one of the prescribed formats that will be described below, and 6) an ending semicolon (;). One reaction line is entered for each chemical reaction in the mechanism. Since line wrapping is allowed, a single reaction definition can span multiple lines in the input file. The generic format for the reaction portion of the reaction line follows,

[<label>] [reac₁[+reac₂[+reac₃]]] = [±[p₁*]prod₁ [±[p₂*]prod₂ [... ± [p₁₂*]prod₁₂]]]

where,
the quantities inside brackets are optional,
reac_n represents a reactant species name,

prod_n a product species name, and
 p_n a stoichiometric coefficient.

Each of the components of the reaction is described below:

- *Labels.* Reaction labels are optional, but highly recommended. They are used to reference specific reactions in some reaction rate forms and may be used by other CMAQ processors, such as the Process Analysis Control Program. As indicated above, they are enclosed by "< >", and any embedded blanks included in the label are omitted from the label.
- *Reactants.* The reactants consist of up to three predefined or user-defined species names separated by plus signs (+). Stoichiometric coefficients are not allowed and are always assumed to equal 1.0. Note that if a predefined species name is used as a reactant, the concentration of that species will be used in determining the rate constant. Since the number of reactants may range from zero to three, reactions from zero order to third order can be included.
- *Products.* The products also consist of a series of predefined or user-defined species names separated by plus (+) or minus (-) signs and optional numerical coefficients. As noted above, up to 12 products may be included, and the stoichiometric coefficients may be either real, integer, or E-format. They must be separated from the species names by an asterisk.

The final part of each reaction line contains the rate constant parameters for the reaction. Rate constant parameters are delimited from the reaction information by either a # sign or a delimiter of the form "%n#", where n is a number (currently 1, 2, or 3). At present, two different photolysis rate forms and ten different thermal rate constant forms can be used, and these are defined in Table M-8. The input value C in this table equals the activation energy (Ea) divided by the gas-law constant R (i.e., $C = \frac{Ea}{R}$). If the activation energy is in units of kcal / mol, then the corresponding value of $R = 0.0019872$ kcal / mol °K. Note that the negative value of C is always used in the exponential expressions. Notes about some of the special forms defined in table M-8 follow.

For photolysis rate reactions, the expressions <J_Label> refers to a label used to identify photolysis rates produced by the CMAQ photolysis rate pre-processor. This processor has been set up to produce photolysis rates for various species in the chemical mechanism. See Table M-9 for a listing of the photolysis rates that can be generated and the valid label names that are assigned to each. If one is not available for a particular species of interest, it is still possible to develop a surrogate rate by selecting an appropriate value of A to scale the available rate to approximate the desired rate.

The expression <k_Label> in photolytic reaction type 2 and thermal reaction types 5 and 6 refers to the labels of other reactions in the mechanism. The term k_n in the corresponding equation refers to the rate constant for the reaction with that label. Thus, for photolytic type 2 and thermal type 6, the effect of using one of these forms is to scale the rate for the reaction to that of another. Thermal reaction

form 5 is a reverse equilibrium reaction form, where A@C is the equilibrium constant and the expression <k_Label> refers to the rate constant for the forward reaction. Note that in thermal reaction type 5 and 6, the symbols E and K must be uppercase.

Finally, P in the equation for thermal reaction type 7 is pressure in atmospheres. Also, the default values for the parameters F and N in thermal reaction rate constant type 10 (i.e., the Falloff expression) are 0.6 and 1.0, respectively. Values need not be specified for these parameters if the defaults are being used. Similarly, the activation energy inputs (@C0 and @C1) do not need to be explicitly included if they are zero.

END keyword. The last entry in the file is the keyword to indicate the end of the mechanism. The first three characters of that keyword must be "END" or "end". Because these characters are used to indicate the end of a mechanism, the first reactant in any reaction cannot begin with these same characters unless it is preceded by a reaction label.

REFERENCES

Gery, M.W. and Crouse, R.R. (1990). User's Guide for Executing OZIPR. EPA/600/8-90, U.S. Environmental Protection Agency, Research Triangle Park, NC 27711.

Jeffries, H.E. (1990). User's Guide to Photochemical Kinetics Simulation System PC-PKSS Software Version 3, Chapel Hill, NC 27514.

Table M-8. Rate Constant Forms

Photolytic Reactions:

Type	Input form	Equation	Example
1	A / <J_label>	$k = A \ J$	# 1.0 / <NO2_CBIV88>;
2	A / <k_label>	$k = A \ k_n$	# 2.0 / <P1>;

Thermal reactions:

Type	Input Form	Equation	Example
1	A	$k = A$	# 9.3E-12;
2	A^B	$k = A (T/300)^B$	# 1.2E-12 ^ -1.3;
3	A@C	$k = A e^{-CT}$	# 1.70E-11 @ 1400.0;
4	A^B@C	$k = A (T/300)^B e^{-CT}$	# 6.165E-13 ^ 2 @ 444.0;
5	A@C^E<k_label>	$k = k_n / (A e^{-CT})$	# 2.1E-27 @ -10900.0 * E<10>;
6	A*K<k_label>	$k = A k_n$	# 2.0E-02 * K <100>;
7	A	$k = A (1.0 + 0.6 P)$	%1 # 1.50E-13;
8	A0@C0&A2&C2@A3@C3	Special Expression 2	%2 # 7.2E-15 @ -785 & 4.1E-16 @ -1440 & 1.9E-33 @ -980.0;
9	A1@C1&A2@C2	Special Expression 3	%3 # 2.2E-13 @ -620.0 & 1.9E-33 @ -980.0;
10	A0^B0@C0&A1^B1@C1&F^N	Falloff Expression	# 1.8E-31 ^ -3.2 & 4.7E-12 ^ -1.4 & 0.6 & 1.0;

Special Expression 2:

$$k_0 = A_0 e^{-C_0/T} \quad k_2 = A_2 e^{-C_2/T} \quad k_3 = A_3 e^{-C_3/T}$$

$$k = k_0 + k_0 [M] / (1 + k_0 [M] / k_0)$$

Special Expression 3:

$$k_1 = A_1 e^{-C_1/T} \quad k_2 = A_2 e^{-C_2/T}$$

$$k = k_1 + k_2 [M]$$

Falloff Expression:

$$k_0 = A_0 (T/300)^{B_0} e^{-C_0/T} \quad k_1 = A_1 (T/300)^{B_1} e^{-C_1/T}$$

$$k = \{k_0 [M] / (1 + k_0 [M] / k_1)\} F^{((1/N) + [\log_{10}(k_0 [M] / k_1)]^2)^{-1}}$$

Table M-9. Photolysis Reaction Mapping to Chemical Mechanisms

Photolysis Reaction	Description	RADM2 Mechanism Label	CB-IV Mechanism Label	SAPRC Mechanism Label	Recent NASA Published Data Label
O2 + hv -> O + O	Molecular Oxygen photolysis	O2_RADM88			O2_NASA94
O3 + hv -> O2 + O(1D)	Ozone Photolysis to O1D	O3O1D_RADM88	O3O1D_CBIV88	O3O1D_SAPRC91	O3O1D_NASA94
O3 + hv > O2 + O(3P)	Ozone Photolysis to O3P	O3O3P_RADM88		O3O3P_SAPRC91	O3O3P_NASA94
NO2 + hv > NO + O	Nitrogen Dioxide Photolysis	NO2_RADM88	NO2_CBIV88	NO2_SAPRC91	NO2_NASA94
NO3 + hv > NO + O2	Nitrate Photolysis to NO	NO3NO_RADM88		NO3NO_SAPRC91	NO3NO_NASA94
NO3 + hv > NO2 + O(3P)	Nitrate Photolysis to NO2	NO3NO2_RADM88		NO3NO2_SAPRC91	NO3NO2_NASA94
HONO + hv > OH + NO	Nitrous Acid Photolysis	HONO_RADM88		HONO_SAPRC91	HONO_NASA94
HNO3 + hv > OH + NO2	Nitric Acid Photolysis	HNO3_RADM88		HNO3_SAPRC91	HNO3_NASA94
HNO4 + hv > HO2 + NO2	Pernitric Acid Photolysis	HNO4_RADM88			HNO4_NASA94
H2O2 + hv > OH + OH	Hydrogen Peroxide Photolysis	H2O2_RADM88		H2O2_SAPRC91	H2O2_NASA94
HCHO + hv > H + HCO	Formaldehyde Photolysis to Radicals	HCHOrad_RADM88	HCHOrad_CBIV88	HCHOrad_SAPRC91	HCHOrad_NASA94
HCHO + hv > H2 + CO	Formaldehyde Photolysis to Molecular Hydrogen	HCHOMol_RADM88	HCHOMol_CBIV88	HCHOMol_SAPRC91	HCHOMol_NASA94
CH3CHO + hv (+2O2) > CH3OO + HO2 + CO	Acetaldehyde Photolysis	ALD_RADM88	ALD_CBIV88	ALD_SAPRC91	
CH3COCH3 + hv > CH3 + CH3CO	Acetone Photolysis	ACETONE_RADM88		ACETONE ???	
CH3COC2H5 + hv > ACO3 + ETH	Methyl Ethyl Ketone Photolysis	KETONE_RADM88		KETONE_SAPRC91	

Photolysis Reaction	Description	RADM2 Mechanism Label	CB-IV Mechanism Label	SAPRC Mechanism Label	Recent NASA Published Data Label
HCOCHO + hv > HCHO + CO	Glyoxal Photolysis to Formaldehyde	GLYform_RADM88			
CH ₃ COCHO + hv > ACO ₃ + HO ₂ + CO	Methyl Glyoxal Photolysis	MGLY_RADM88		MGLY_SAPRC91	
HCOCH=CHCHO + hv > 0.98HO ₂ + TCO ₃ + 0.02ACO ₃	Unsaturated Dicarbonyl Photolysis	UDC_RADM88			
CH ₃ OOH + hv > products	Methyl Hydrogen Peroxide Photolysis	MHP_RADM88		MHP_SAPRC91	MHP_NASA94
CH ₃ ONO ₂ + hv > 0.2ALD + 0.8KET + HO ₂ + NO ₂	Organic Nitrate Photolysis	ORGNIT_RADM88			
HCOCHO + hv > 2CO + H ₂	Glyoxal Photolysis to Molecular Hydrogen	GLYmol_RADM88			
RCHO + hv > CCHO + RO ₂ R + RO ₂ + CO + HO ₂	Propionaldehyde Photolysis			PROPA_SAPRC91	
AFG2 + hv > HO ₂ + CO + CCO O ₂ + RCO ₃	Unknown Aromatic Ring Fragment Photolysis			UARF_SAPRC91	
C ₃ H ₄ O + hv -> products	Acrolein Photolysis	ACROLEIN	ACROLEIN		

Example M-1. CB4 Mechanism Listing

```

! Created by Jerry Gipson, May, 1997
! The reaction labels correspond to those used in "A Photochemical Kinetics
! Mechanism for Urban and Regional Scale Computer Modeling" M. Gery et al.
! (JGR, 9/89) and to the numbers assigned to reactions in the UAM-V model
! for new reactions. Reactions of methanol and ethanol are optional
! in UAM, and thus are commented out in this version. They need to be
! "un-commented" if they are to be included. See Volume 6 for a description
! of the changes that have been made to the original version.

! Modified by Jerry Gipson 3/98 to update isoprene chemistry to Carter's
! one product form, to change CO rate constant to the pressure dependent
! form, and to correct miscellaneous typos.

! Modified by Jerry Gipson 3/98 to track all stable nitrogen products as
! AACD - Acetic and higher acids
! PACD - Peroxy acetic acid
! UMHP - Upper limit estimate of methylhydroperoxide

```

CB4.2

REACTIONS[CM] =

< R1> NO2	=	NO + O	# 1.0 /<NO2_CBIV88>;
< R2> O + O2	=	O3	# 6.0E-34 ^ -2.3 & 2.8E-12;
< R3> O3 + NO	=	NO2	# 1.8E-12 @ 1370;
< R4> O + NO2	=	NO	# 9.3E-12;
< R5> O + NO2	=	NO3	# 9.0E-32 ^ -2.0 & 2.2E-11;
< R6> O + NO	=	NO2	# 9.0E-32 ^ -1.5 & 3.0E-11;
< R7> O3 + NO2	=	NO3	# 1.2E-13 @ 2450;
< R8> O3	=	O	# 0.053 / <NO2_CBIV88>;
< R9> O3	=	O1D	# 1.0 / <O3O1D_CBIV88>;
<R10a> O1D + N2	=	O	# 1.8E-11 @ -107;
<R10b> O1D + O2	=	O	# 3.2E-11 @ -67;
< R11> O1D + H2O	=	2.0*OH	# 2.2E-10;
< R12> O3 + OH	=	HO2	# 1.6E-12 @ 940;
< R13> O3 + HO2	=	OH	# 1.4E-14 @ 580;
< R14> NO3	=	0.89*NO2 + 0.89*O + 0.11*NO	# 33.9 / <NO2_CBIV88>;
< R15> NO3 + NO	=	2.0*NO2	# 1.3E-11 @ -250;
< R16> NO3 + NO2	=	NO + NO2	# 2.5E-14 @ 1230;
< R17> NO3 + NO2	=	N2O5	# 2.2E-30 ^ -4.3 & 1.5E-12 ^ -0.5;
< R18> N2O5 + H2O	=	2.0*HNO3	# 1.3E-21;
< R19> N2O5	=	NO3 + NO2	# 3.5E+14 @ 10897;
< R20> NO + NO + O2	=	2.0*NO2	# 3.3E-39 @ -530;
< R21> NO + NO2 + H2O	=	2.000*HONO	# 4.4E-40;
< R22> OH + NO	=	HONO	# 6.7E-31 ^ -3.3 & 3.0E-11 ^ -1.0;
< R23> HONO	=	OH + NO	# 0.1975 / <NO2_CBIV88>;
< R24> HONO + OH	=	NO2	# 6.6E-12;
< R25> HONO + HONO	=	NO + NO2	# 1.0E-20;

< R26> OH + NO2 = HNO3 # 2.6E-30 ^ -3.2 &
 2.4E-11 ^ -1.3;

 < R27> OH + HNO3 = NO3 %2 # 7.2E-15 @ -785 &
 4.1E-16 @ -1440 &
 1.9E-33 @ -725;

 < R28> HO2 + NO = OH + NO2 # 3.7E-12 @ -240;

 < R29> HO2 + NO2 = PNA # 2.3E-31 ^ -4.6 &
 4.2E-12 ^ 0.2;

 < R30> PNA = HO2 + NO2 # 4.8E+13 @ 10121;
 < R31> PNA + OH = NO2 # 1.3E-12 @ -380;
 < R32> HO2 + HO2 = H2O2 # 5.9E-14 @ -1150;
 < R33> HO2 + HO2 + H2O = H2O2 # 2.2E-38 @ -5800;
 < R34> H2O2 = 2*OH # 0.255 / <HCHOmol_CBIV88>;
 < R35> H2O2 + OH = HO2 # 3.1E-12 @ 187;
 < R36> CO + OH = HO2 # 1.5E-13;
 < R37> FORM + OH = HO2 + CO # 1.0E-11;
 < R38> FORM = 2*HO2 + CO # 1.0 / <HCHO_rad_CBIV88>;
 < R39> FORM = CO # 1.0 / <HCHOmol_CBIV88>;
 < R40> FORM + O = OH + HO2 + CO # 3.0E-11 @ 1550;
 < R41> FORM + NO3 = HNO3 + HO2 + CO # 6.3E-16;
 < R42> ALD2 + O = C2O3 + OH # 1.2E-11 @ 986;
 < R43> ALD2 + OH = C2O3 # 7.0E-12 @ -250;
 < R44> ALD2 + NO3 = C2O3 + HNO3 # 2.5E-15;
 < R45> ALD2 = XO2 + 2*HO2 + CO + FORM # 1.0 / <ALD_CBIV88>;
 < R46> C2O3 + NO = NO2 + XO2 + FORM + HO2 # 3.49E-11 @ 180;
 < R47> C2O3 + NO2 = PAN # 2.63E-12 @ -380;
 < R48> PAN = C2O3 + NO2 # 2.00E+16 @ 13500;
 < R49> C2O3 + C2O3 = 2*XO2 + 2*FORM + 2*HO2 # 2.5E-12;
 < R50> C2O3 + HO2 = 0.79*FORM + 0.79*XO2 +
 0.79*HO2 + 0.79*OH +
 0.21*PACD # 6.5E-12;

 < R51> {CH4 +} OH = XO2 + FORM + HO2 # 1.1E+02 @ 1710;

 < R52> PAR + OH = 0.87*XO2 + 0.13*XO2N +
 0.11*HO2 + 0.11*ALD2 +
 0.76*ROR - 0.11*PAR # 8.1E-13;

 < R53> ROR = 1.1*ALD2 + 0.96*XO2 +
 0.94*HO2 - 2.10*PAR +
 0.04*XO2N + 0.02*ROR # 1.0E+15 @ 8000;

 < R54> ROR = HO2 # 1.6E+03;
 < R55> ROR + NO2 = NTR # 1.5E-11;

 < R56> OLE + O = 0.63*ALD2 + 0.38*HO2 +
 0.28*XO2 + 0.3*CO +
 0.2*FORM + 0.02*XO2N +
 0.22*PAR + 0.2*OH # 1.2E-11 @ 324;

 < R57> OLE + OH = FORM + ALD2 + XO2 +
 HO2 - PAR # 5.2E-12 @ -504;

 < R58> OLE + O3 = 0.5*ALD2 + 0.74*FORM +
 0.33*CO + 0.44*HO2 +

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          0.22*XO2 + 0.1*OH +
          0.20*FACD + 0.20*AACD -
          PAR                                         # 1.4E-14 @ 2105;

< R59> OLE + NO3      = 0.91*XO2 + 0.09*XO2N +
          FORM + ALD2 - PAR + NO2                 # 7.7E-15;

< R60> ETH + O        = FORM + 0.7*XO2 + CO +
          1.7*HO2 + 0.3*OH                         # 1.0E-11 @ 792;

< R61> ETH + OH       = XO2 + 1.56*FORM + HO2 +
          0.22*ALD2                                    # 2.0E-12 @ -411;

< R62> ETH + O3       = FORM + 0.42*CO + 0.12*HO2 +
          0.40*FACD                                    # 1.3E-14 @ 2633;

< R63> TOL + OH       = 0.08*XO2 + 0.36*CRES +
          0.44*HO2 + 0.56*TO2 + TOLAER
                                         # 2.1E-12 @ -322;

< R64> TO2 + NO       = 0.9*NO2 + 0.9*HO2 +
          0.9*OPEN + 0.1*NTR                        # 8.1E-12;

< R65> TO2              = CRES + HO2                  # 4.2;

< R66> CRES + OH       = 0.4*CRO + 0.6*XO2 +
          0.6*HO2 + 0.3*OPEN + CSLAER
                                         # 4.1E-11;

< R67> CRES + NO3     = CRO + HNO3 + CSLAER
                                         # 2.2E-11;

< R68> CRO + NO2       = NTR                      # 1.4E-11;

< R69> XYL + OH        = 0.7*HO2 + 0.5*XO2 +
          0.2*CRES + 0.8*MGLY +
          1.1*PAR + 0.3*TO2 + XYLAER
                                         # 1.7E-11 @ -116;

< R70> OPEN + OH       = XO2 + 2*CO + 2*HO2 +
          C2O3 + FORM                                # 3.0E-11;

< R71> OPEN              = C2O3 + HO2 + CO
                                         # 9.04 /<HCHOrad_CBIV88>;

< R72> OPEN + O3        = 0.03*ALD2 + 0.62*C2O3 +
          0.7*FORM + 0.03*XO2 +
          0.69*CO + 0.08*OH +
          0.76*HO2 + 0.2*MGLY
                                         # 5.4E-17 @ 500;

< R73> MGLY + OH       = XO2 + C2O3                  # 1.7E-11;

< R74> MGLY              = C2O3 + HO2 + CO
                                         # 9.64 / <HCHOrad_CBIV88>;

< R75> ISOP + O         = 0.75*ISPD + 0.50*FORM +
          0.25*XO2 + 0.25*HO2 +
          0.25*C2O3 + 0.25*PAR
                                         # 3.6E-11;

< R76> ISOP + OH       = 0.912*ISPD + 0.629*FORM +
          0.991*XO2 + 0.912*HO2 +
          0.088*XO2N
                                         # 2.54E-11 @ -407.6;

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< R77> ISOP + O3      = 0.65*ISPD + 0.60*FORM +
                           0.20*XO2 + 0.066*HO2 +
                           0.266*OH + 0.20*C2O3 +
                           0.15*ALD2 + 0.35*PAR +
                           0.066*CO
                                         # 7.86E-15 @ 1912;

< R78> ISOP + NO3     = 0.20*ISPD + 0.80*NTR +
                           1.0*XO2 + 0.80*HO2 +
                           0.20*NO2 + 0.80*ALD2 +
                           2.4*PAR
                                         # 3.03E-12 @ 448;

< R79> XO2 + NO       = NO2
< R80> XO2 + XO2      =
< R81> XO2N + NO      = NTR
< R82> SO2 + OH       = SULF + HO2 + SULAER
< R83> SO2             = SULF + SULAER
!< R84> MEOH + OH     =
!< R85> ETOH + OH     =
< R86> XO2 + HO2      = UMHP
< R87> XO2N + HO2     =
< R88> XO2N + XO2N    =
< R89> XO2N + XO2     =
                                         # 8.1E-12;
                                         # 1.7E-14 @ -1300;
                                         # 8.12E-12;
                                         # 4.39E-13 @ -160;
                                         # 1.36E-06;
                                         # 1.08E-12;
                                         # 1.61E-12 @ -176;
                                         # 7.67E-14 @ -1300.0;
                                         # 7.67E-14 @ -1300.0;
                                         # 1.73E-14 @ -1300.0;
                                         # 3.45E-14 @ -1300.0;

< R90> ISPD + OH      = 1.565*PAR + 0.167*FORM +
                           0.713*XO2 + 0.503*HO2 +
                           0.334*CO + 0.168*MGLY +
                           0.273*ALD2 + 0.498*C2O3
                                         # 3.36E-11;

< R91> ISPD + O3      = 0.114*C2O3 + 0.150*FORM +
                           0.850*MGLY + 0.154*HO2 +
                           0.268*OH + 0.064*XO2 +
                           0.020*ALD2 + 0.360*PAR +
                           0.225*CO
                                         # 7.11E-18;

< R92> ISPD + NO3     = 0.357*ALD2 + 0.282*FORM +
                           1.282*PAR + 0.925*HO2 +
                           0.643*CO + 0.850*NTR +
                           0.075*C2O3 + 0.075*XO2 +
                           0.075*HNO3
                                         # 1.00E-15;

< R93> ISPD            = 0.333*CO + 0.067*ALD2 +
                           0.900*FORM + 0.832*PAR +
                           1.033*HO2 + 0.700*XO2 +
                           0.967*C2O3
                                         # 0.0036 / <ACROLEIN>;

< R94> ISOP + NO2     = 0.20*ISPD + 0.80*NTR +
                           1.00*XO2 + 0.80*HO2 +
                           0.20*NO + 0.80*ALD2 +
                           2.4*PAR
                                         # 1.49E-19;

< AE1> TERP + OH      = TERPAER + OH
< AE1> TERP + NO3     = TERPAER + NO3
< AE1> TERP + O3      = TERPAER + O3
                                         # 1.07E-11 @ -549.0;
                                         # 3.23E-11 @ 975.0;
                                         # 7.29E-15 @ 1136.0;

```

END MECH

Example M-2. RADM2 Mechanism Listing

```

! RADM2 Mechanism originally based on OZIPR version and modified
! to be consistent with the RADM2 mechanism embedded in
! version h26.f of HR-RADM. Reaction labels below correspond
! to the reaction numbers in the HR-RADM model. (Note: Reaction 40
! in the original RADM mechanism is represented by reactions 40 and
! 40a below.) Jeff & Jerry 23 Aug 96

```

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! Modified by Jerry Gipson 3/12/97 to include gaseous species that
! are necessary to link gas-phase chemistry to aerosol formation.

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! New species added:

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! SULAER: Gives amount of sulfuric acid produced
! TOLAER: Gives total amount of TOL reacted
! XYLAER: Gives total amount of XYL reacted
! CSLAER: Gives total amount of CSL reacted
! HC8AER: Gives total amount of HC8 reacted
! OLIAER: Gives total amount of OLI reacted
! TERP: Monoterpenes
! TERPAER: Gives total amount of monoterpenes reacted
! Three new reactions were added: AE1 AE2 and AE3

```

RADM2

REACTIONS [cm] =

```

< P1> NO2      =     O3P    +    NO      # 1.0 /<NO2_RADM88>;
< P2> O3        =     O1D    +      # 1.0 /<O3O1D_RADM88>;
< P3> O3        =     O3P    +      # 1.0 /<O3O3P_RADM88>;
< P4> HONO      =     HO    +    NO      # 1.0 /<HONO_RADM88>;
< P5> HNO3      =     HO    +    NO2     # 1.0 /<HNO3_RADM88>;
< P6> HNO4      =     HO2   +    NO2     # 1.0 /<HNO4_RADM88>;
< P7> NO3       =     NO      +      # 1.0 /<NO3NO_RADM88>;
< P8> NO3       =     NO2   +     O3P     # 1.0 /<NO3NO2_RADM88>;
< P9> H2O2      = 2.0* HO      +      # 1.0 /<H2O2_RADM88>;
< P10> HCHO      =     CO      +      # 1.0
/<HCHOmol_RADM88>;
< P11> HCHO      =     HO2   +    HO2   +    CO      # 1.0
/<HCHOrad_RADM88>;
< P12> ALD      =     MO2   +    HO2   +    CO      # 1.0 /<ALD_RADM88>;
< P13> OP1      =     HCHO  +    HO2   +    HO      # 1.0 /<MHP_RADM88>;
< P14> OP2      =     ALD   +    HO2   +    HO      # 1.0 /<HOP_RADM88>;
< P15> PAA      =     MO2   +    HO      +      # 1.0 /<PAA_RADM88>;
< P16> KET      =     ACO3  +    ETHP     +      # 1.0 /<KETONE_RADM88>;
< P17> GLY      = 0.13*HCHO + 1.870*CO      +      # 1.0
/<GLYform_RADM88>;
< P18> GLY      = 0.45*HCHO + 1.550*CO + 0.800*HO2 # 1.0 /<GLYmol_RADM88>;
< P19> MGLY      =     ACO3  +    HO2   +    CO      # 1.0 /<MGLY_RADM88>;
< P20> DCB      = 0.98*HO2 + 0.020*ACO3 + TCO3 # 1.0 /<UDC_RADM88>;
< P21> ONIT      = 0.20*ALD + 0.800*KET + HO2 + NO2 # 1.0 /<ORGNIT_RADM88>;
< 1> O3P + O2 + M =     O3      +      # 6.0E-34^-2.3;
< 2> O3P + NO2 =     NO      +      # 6.5E-12 @ -120.0;
< 3> O1D + N2 =     O3P      +      # 1.8E-11 @ -110.0;
< 4> O1D + O2 =     O3P      +      # 3.2E-11 @ -70.0;
< 5> O1D + H2O = 2.0* HO      +      # 2.20E-10;
< 6> O3 + NO =     NO2      +      # 2.00E-12 @1400.0;
< 7> O3 + HO =     HO2      +      # 1.60E-12 @ 940.0;
< 8> O3 + HO2 =     HO      +      # 1.10E-14 @ 500.0;
< 9> HO2 + NO =     NO2      +    HO      # 3.70E-12 @ -240.0;
< 10> HO2 + NO2 =     HNO4     +      # 1.8E-31^-3.2 &4.7E-12^-1.4;

```

< 11> HNO4 = HO2 + NO2 # 2.1E-27 @ -10900.0 *E< 10>;
 < 12> HO2 + HO2 = H2O2 %3 # 2.20E-13@-620.0 & 1.90E-33@-980.0;
 < 13> HO2 + HO2 + H2O = H2O2 %3 # 3.08E-34@-2820.0 &
 2.66E-54@-3180.0;
 < 14> H2O2 + HO = HO2 # 3.300E-12 @ 200.0;
 < 15> NO + HO = HONO # 7.0E-31^2.6 &1.5E-11^0.5;
 < 16> NO + NO + O2 = 2.0*NO2 # 3.300E-39 @ -530.0;
 < 17> O3 + NO2 = NO3 # 1.4000E-13 @ 2500.0;
 < 18> NO3 + NO = 2.0*NO2 # 1.7000E-11 @ -150.0;
 < 19> NO3 + NO2 = NO + NO2 # 2.5000E-14 @ 1230.0;
 < 20> NO3 + HO2 = HNO3 # 2.5000E-12;
 < 21> NO3 + NO2 = N2O5 # 2.2E-30^4.3 &1.5E-12^0.5;
 < 22> N2O5 = NO2 + NO3 # 1.10E-27 @ -11200.0 *E<21>;
 < 23> N2O5 + H2O = 2.0*HNO3 # 2.00E-21;
 < 24> HO + NO2 = HNO3 # 2.6E-30^3.2 &2.4E-11^1.3;
 < 25> HO + HNO3 = NO3 %2
 #7.2E-15@-785&4.1E-16@-1440&1.9E-33@-725;
 < 26> HO + HNO4 = NO2 # 1.3000E-12 @ -380.0;
 < 27> HO + HO2 = # 4.6000E-11 @ -230.0;
 < 28> HO + SO2 = SULF + HO2 + SULAER # 3.0E-31^3.3 &1.5E-12^0.0;
 < 29> CO + HO = HO2 %1 #1.5000E-13;
 < 30> HO = MO2 (X 300 SQUARED) # 28.3^2 @ 1280.0;
 < 31> ETH + HO = ETHP (X 300 SQUARED) # 1.233E-12^2 @ 444.0;
 < 32> HC3 + HO = 0.83*HC3P + 0.17*HO2 + 0.009*HCHO + 0.075*ALD
 + 0.025*KET # 1.59E-11 @ 540.0;
 < 33> HC5 + HO = HC5P + 0.250*XO2 # 1.73E-11 @ 380.0;
 < 34> HC8 + HO = HC8P + 0.750*XO2 + HC8AER # 3.64E-11 @ 380.0;
 < 35> OL2 + HO = OL2P # 2.15E-12 @ -411.0;
 < 36> OLT + HO = OLTP # 5.32E-12 @ -504.0;
 < 37> OLI + HO = OLIP + OLIAER # 1.07E-11 @ -549.0;
 < 38> TOL + HO = 0.75*TOLP + 0.250*CSL + 0.250*HO2
 + TOLAER # 2.10E-12 @ -322.0;
 < 39> XYL + HO = 0.83*XYLP + 0.170*CSL + 0.170*HO2
 + XYLAER # 1.89E-11 @ -116.0;
 < 40> CSL + HO = 0.10*HO2 + 0.900*XO2 + 0.900*TCO3
 + CSLAER # 4.00E-11;
 <40a> CSL + HO = CSL # 0.9*K<40>;
 < 41> HCHO + HO = HO2 + CO # 9.0000E-12;
 < 42> ALD + HO = ACO3 # 6.8700E-12 @ -256.0;
 < 43> KET + HO = KETP # 1.2000E-11 @ 745.0;
 < 44> GLY + HO = HO2 + 2.000*CO # 1.1500E-11;
 < 45> MGLY + HO = ACO3 + CO # 1.7000E-11;
 < 46> DCB + HO = TCO3 # 2.8E-11;
 < 47> OP1 + HO = 0.5*MO2 + 0.500*HCHO + 0.500*HO # 1.0000E-11;
 < 48> OP2 + HO = 0.5*HC3P + 0.500*ALD + 0.500*HO # 1.0000E-11;
 < 49> PAA + HO = ACO3 # 1.0000E-11;
 < 50> PAN + HO = HCHO + NO3 + XO2 (x 300 sq) # 6.1650E-13^2 @
 444.0;
 < 51> ONIT + HO = HC3P + NO2 # 1.5500E-11 @ 540.0;
 < 52> ISO + HO = OLTP # 2.5500E-11 @ -409.0;
 < 53> ACO3 + NO2 = PAN # 2.8000E-12 @ -181.0;
 < 54> PAN = ACO3 + NO2 # 1.9500E+16 @
 13543.0;
 < 55> TCO3 + NO2 = TPAN # 4.7000E-12;
 < 56> TPAN = TCO3 + NO2 # 1.9500E+16 @
 13543.0;
 < 57> MO2 + NO = HCHO + HO2 + NO2 # 4.2000E-12 @ -180.0;
 < 58> HC3P + NO = 0.75*ALD + 0.25*KET + 0.09*HCHO
 + 0.964*NO2 + 0.964*HO2 # 4.2000E-12 @ -180.0;

< 60> HC5P + NO = 0.38*ALD + 0.69*KET + 0.08*ONIT
 + 0.92*NO2 + 0.92*HO2 # 4.2000E-12 @ -180.0;
 < 62> HC8P + NO = 0.35*ALD + 1.06*KET + 0.04*HCHO
 + 0.24*ONIT + 0.76*NO2 + 0.76*HO2 # 4.2000E-12 @ -180.0;
 < 64> OL2P + NO = 1.6*HCHO + HO2 + NO2 + 0.20*ALD # 4.2000E-12 @ -180.0;
 < 65> OLTP + NO = ALD + HCHO + HO2 + NO2 # 4.2000E-12 @ -180.0;
 < 66> OLIP + NO = HO2 + 1.45*ALD + 0.28*HCHO
 + 0.1*KET + NO2 # 4.2000E-12 @ -180.0;
 < 67> ACO3 + NO = MO2 + NO2 # 4.2000E-12 @ -180.0;
 < 68> TCO3 + NO = NO2 + 0.920*HO2 + 0.890*GLY + 0.110*MGLY
 + 0.050*ACO3 + 0.950*CO + 2.000*XO2 # 4.2000E-12 @ -180.0;
 < 69> TOLP + NO = NO2 + HO2 + 0.17*MGLY
 + 0.16*GLY + 0.70*DCB # 4.2000E-12 @ -180.0;
 < 70> XYLP + NO = NO2 + HO2 + .45*MGLY + .806*DCB # 4.2000E-12 @ -180.0;
 < 71> ETHEP + NO = ALD + HO2 + NO2 # 4.2000E-12 @ -180.0;
 < 72> KETP + NO = MGLY + NO2 + HO2 # 4.2000E-12 @ -180.0;
 < 73> OLN + NO = HCHO + ALD + 2.0*NO2 # 4.2000E-12 @ -180.0;
 < 74> HCHO + NO3 = HO2 + HNO3 + CO # 6.000E-13 @ 2058.0;
 < 75> ALD + NO3 = ACO3 + HNO3 # 1.400E-12 @ 1900.0;
 < 76> GLY + NO3 = HNO3 + HO2 + 2.000*CO # 6.000E-13 @ 2058.0;
 < 77> MGLY + NO3 = HNO3 + ACO3 + CO # 1.400E-12 @ 1900.0;
 < 78> DCB + NO3 = HNO3 + TCO3 # 1.400E-12 @ 1900.0;
 < 79> CSL + NO3 = HNO3 + XNO2 + 0.500*CSL
 + 0.500*CSLAER # 2.200E-11;
 < 80> OL2 + NO3 = OLN # 2.000E-12 @ 2923.0;
 < 81> OLT + NO3 = OLN # 1.000E-11 @ 1895.0;
 < 82> OLI + NO3 = OLN + OLIAER # 3.230E-11 @ 975.0;
 < 83> ISO + NO3 = OLN # 5.810E-13;
 < 84> OL2 + O3 = HCHO + 0.400*ORA1 + 0.420*CO
 + 0.120*HO2 # 1.200E-14 @ 2633.0;
 < 85> OLT + O3 = 0.53*HCHO + 0.500*ALD + 0.33*CO + 0.20*ORA1
 + 0.20*ORA2 + 0.23*HO2 + 0.22*MO2 + 0.10*HO
 # 1.3200E-14 @ 2105.0;
 < 86> OLI + O3 = 0.18*HCHO + 0.72*ALD + 0.10*KET + 0.23*CO + 0.06*ORA1
 + 0.29*ORA2 + 0.26*HO2 + 0.14*HO + 0.31*MO2
 + OLIAER # 7.2900E-15 @ 1136.0;
 < 87> ISO + O3 = 0.53*HCHO + 0.500*ALD + 0.33*CO + 0.20*ORA1
 + 0.20*ORA2 + 0.23*HO2 + 0.22*MO2 + 0.10*HO
 # 1.230E-14 @ 2013.0;
 < 88> HO2 + MO2 = OP1 # 7.700E-14 @ -1300.0;
 < 89> HO2 + ETHEP = OP2 # 7.700E-14 @ -1300.0;
 < 90> HO2 + HC3P = OP2 # 7.700E-14 @ -1300.0;
 < 91> HO2 + HC5P = OP2 # 7.700E-14 @ -1300.0;
 < 92> HO2 + HC8P = OP2 # 7.700E-14 @ -1300.0;
 < 93> HO2 + OL2P = OP2 # 7.700E-14 @ -1300.0;
 < 94> HO2 + OLTP = OP2 # 7.700E-14 @ -1300.0;
 < 95> HO2 + OLIP = OP2 # 7.700E-14 @ -1300.0;
 < 96> HO2 + KETP = OP2 # 7.700E-14 @ -1300.0;
 < 97> HO2 + ACO3 = PAA # 7.700E-14 @ -1300.0;
 < 98> HO2 + TOLP = OP2 # 7.700E-14 @ -1300.0;
 < 99> HO2 + XYLP = OP2 # 7.700E-14 @ -1300.0;
 <100> HO2 + TCO3 = OP2 # 7.700E-14 @ -1300.0;
 <101> HO2 + OLN = ONIT # 7.700E-14 @ -1300.0;
 <102> MO2 + MO2 = 1.5*HCHO + HO2 # 1.90E-13 @ -220.0;
 <103> MO2 + ETHEP = 0.75*HCHO + HO2 + 0.75*ALD # 1.40E-13 @ -220.0;
 <104> MO2 + HC3P = 0.84*HCHO + 0.770*ALD + 0.260*KET
 + 1.000*HO2 # 4.20E-14 @ -220.0;
 <105> MO2 + HC5P = 0.77*HCHO + 0.41*ALD + 0.75*KET

$ \begin{aligned} & + 1.000 * \text{HO}_2 \\ <106> \text{MO}_2 + \text{HC8P} = & 0.80 * \text{HCHO} + 0.46 * \text{ALD} + 1.39 * \text{KET} \\ & + 1.000 * \text{HO}_2 \\ <107> \text{MO}_2 + \text{OL2P} = & 1.55 * \text{HCHO} + 0.350 * \text{ALD} + \text{HO}_2 \\ <108> \text{MO}_2 + \text{OLTP} = & 1.25 * \text{HCHO} + 0.750 * \text{ALD} + \text{HO}_2 \\ <109> \text{MO}_2 + \text{OLIP} = & 0.89 * \text{HCHO} + 0.725 * \text{ALD} + \text{HO}_2 \\ & + 0.55 * \text{KET} \\ <110> \text{MO}_2 + \text{KETP} = & 0.75 * \text{HCHO} + 0.750 * \text{MGLY} + \text{HO}_2 \\ <111> \text{MO}_2 + \text{ACO3} = & \text{HCHO} + 0.5 * \text{HO}_2 + 0.5 * \text{MO}_2 \\ & + 0.50 * \text{ORA2} \\ <112> \text{MO}_2 + \text{TOLP} = & \text{HCHO} + 0.17 * \text{MGLY} + 0.16 * \text{GLY} \\ & + 0.70 * \text{DCB} + 2.0 * \text{HO}_2 \\ <113> \text{MO}_2 + \text{XYLP} = & \text{HCHO} + 0.45 * \text{MGLY} + 0.806 * \text{DCB} \\ & + 2.000 * \text{HO}_2 \\ <114> \text{MO}_2 + \text{TCO3} = & .50 * \text{HCHO} + 0.445 * \text{GLY} + 0.055 * \text{MGLY} \\ & + 0.50 * \text{ORA2} + 0.025 * \text{ACO3} + 0.460 * \text{HO}_2 \\ & + 0.475 * \text{CO} + \text{XO}_2 \\ <138> \text{MO}_2 + \text{OLN} = & 1.75 * \text{HCHO} + 0.50 * \text{HO}_2 + \text{ALD} + \text{NO}_2 \\ <115> \text{ETHP} + \text{ACO3} = & \text{ALD} + 0.5 * \text{HO}_2 + 0.5 * \text{MO}_2 \\ & + 0.5 * \text{ORA2} \\ <116> \text{HC3P} + \text{ACO3} = & .77 * \text{ALD} + 0.26 * \text{KET} + 0.5 * \text{HO}_2 \\ & + 0.50 * \text{MO}_2 + 0.5 * \text{ORA2} \\ <117> \text{HC5P} + \text{ACO3} = & 0.41 * \text{ALD} + 0.75 * \text{KET} + 0.5 * \text{HO}_2 \\ & + 0.50 * \text{MO}_2 + 0.5 * \text{ORA2} \\ <118> \text{HC8P} + \text{ACO3} = & 0.46 * \text{ALD} + 1.39 * \text{KET} + 0.5 * \text{HO}_2 \\ & + 0.50 * \text{MO}_2 + 0.5 * \text{ORA2} \\ <119> \text{OL2P} + \text{ACO3} = & 0.80 * \text{HCHO} + 0.6 * \text{ALD} + 0.5 * \text{HO}_2 \\ & + 0.5 * \text{MO}_2 + 0.5 * \text{ORA2} \\ <120> \text{OLTP} + \text{ACO3} = & \text{ALD} + 0.5 * \text{HCHO} + 0.5 * \text{HO}_2 \\ & + 0.5 * \text{MO}_2 + 0.5 * \text{ORA2} \\ <121> \text{OLIP} + \text{ACO3} = & 0.725 * \text{ALD} + 0.55 * \text{KET} + 0.14 * \text{HCHO} \\ & + 0.5 * \text{HO}_2 + 0.50 * \text{MO}_2 + 0.5 * \text{ORA2} \\ <122> \text{KETP} + \text{ACO3} = & \text{MGLY} + 0.5 * \text{HO}_2 + 0.5 * \text{MO}_2 \\ & + 0.5 * \text{ORA2} \\ <123> \text{ACO3} + \text{ACO3} = & 2.0 * \text{MO}_2 \\ <124> \text{ACO3} + \text{TOLP} = & \text{MO}_2 + 0.170 * \text{MGLY} + 0.16 * \text{GLY} \\ & + 0.70 * \text{DCB} + \text{HO}_2 \\ <125> \text{ACO3} + \text{XYLP} = & \text{MO}_2 + 0.45 * \text{MGLY} + 0.806 * \text{DCB} \\ & + \text{HO}_2 \\ <126> \text{ACO3} + \text{TCO3} = & \text{MO}_2 + 0.92 * \text{HO}_2 + 0.89 * \text{GLY} \\ & + 0.11 * \text{MGLY} + 0.05 * \text{ACO3} + 0.95 * \text{CO} \\ & + 2.0 * \text{XO}_2 \\ <139> \text{ACO3} + \text{OLN} = & \text{HCHO} + \text{ALD} + 0.5 * \text{ORA2} \\ & + \text{NO}_2 + 0.5 * \text{MO}_2 \\ <140> \text{OLN} + \text{OLN} = & 2.0 * \text{HCHO} + 2.0 * \text{ALD} + 2.0 * \text{NO}_2 \end{aligned} $	$ \begin{aligned} & \# 3.40\text{E-}14 @ -220.0; \\ & \# 2.90\text{E-}14 @ -220.0; \\ & \# 1.40\text{E-}13 @ -220.0; \\ & \# 1.40\text{E-}13 @ -220.0; \\ & \# 1.70\text{E-}14 @ -220.0; \\ & \# 1.70\text{E-}14 @ -220.0; \\ & \# 9.60\text{E-}13 @ -220.0; \\ & \# 1.70\text{E-}14 @ -220.0; \\ & \# 1.70\text{E-}14 @ -220.0; \\ & \# 9.60\text{E-}13 @ -220.0; \\ & \# 1.70\text{E-}14 @ -220.0; \\ & \# 3.40\text{E-}13 @ -220.0; \\ & \# 1.00\text{E-}13 @ -220.0; \\ & \# 8.40\text{E-}14 @ -220.0; \\ & \# 7.20\text{E-}14 @ -220.0; \\ & \# 3.40\text{E-}13 @ -220.0; \\ & \# 3.40\text{E-}13 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 1.19\text{E-}12 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 1.19\text{E-}12 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 7.70\text{E-}14 @ -1300.0; \\ & \# 1.70\text{E-}14 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 3.60\text{E-}16 @ -220.0; \\ & \# 4.2000\text{E-}12 @ -180.0; \\ & \# 4.2000\text{E-}12 @ -180.0; \\ & \# 7.70\text{E-}14 @ -1300.0; \\ & \# 1.70\text{E-}14 @ -220.0; \\ & \# 4.20\text{E-}14 @ -220.0; \\ & \# 3.60\text{E-}16 @ -220.0; \\ & \# 1.0 * \text{K} < 37 >; \\ & \# 1.0 * \text{K} < 82 >; \\ & \# 1.0 * \text{K} < 86 >; \end{aligned} $
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endmech

Process Analysis (PROCAN)

Introduction. Process Analysis is a diagnostic tool that captures model-generated data not routinely output by models and provides quantitative information on the contributions of individual physical and chemical processes to model predictions. This quantitative information can then be used to form a picture of how the model obtains its predictions. In the CMAQ modeling system, two types of Process Analysis data can be captured during a CCTM simulation: IPRs and IRRs. IPRs give the contributions of individual physical processes and the net effect of chemical reactions to the overall model concentrations. IRRs give the contributions of individual chemical reactions to the net effects of chemical reaction on species concentrations. Because the amount of IPR and IRR data that can be obtained may be large and the analysis of such data can be fairly complex, the user is advised to read Chapter 17 in the *Models-3 Volume 6b: Science of the Community Multi-scale Air Quality (CMAQ) Modeling System* before attempting to use this tool. The discussion here focuses primarily on the procedures that must be followed to capture Process Analysis data rather than on what data should be captured and how it might be analyzed.

As noted in Section 11.4.1 of this User's Guide, all of the predefined mechanisms have been set up to omit process analysis. If process analysis is to be invoked using one of the predefined mechanisms, it will be necessary to modify the mechanism in the Models-3 Chemical Mechanism Manager. That chemical mechanism will then have to be assigned a new name to reflect the addition of process analysis. See the section on modifying a chemical mechanism for the procedures to follow. The process analysis data themselves are entered by selecting the *Process Analysis* tab in the Chemical Mechanism Manager. As described in Section 7.5.2, the process analysis inputs consist of a series of commands that can be entered directly in the window or can be imported into the framework via an ASCII text file. Since the process analysis commands can be somewhat lengthy, the latter approach is recommended. The ASCII file can be created with any editor or word processor that generates a standard ASCII file.

The commands in a command file are processed transparently in the Models-3 framework by the PACP. This program reads and interprets the commands and then generates three include files (.ext) used by CCTM to produce the Process Analysis outputs that were requested in the commands. These include files are automatically made available to the Model Builder for inclusion in the configuration file used to make an executable with your requested process analysis. Since this is handled automatically within the framework, you need only concern yourself with developing the appropriate input PACP commands. In this appendix, refer to Example M-3 of an input command file and a corresponding output report PA_REPORT (Example M-4) generated by the PACP. You may wish to refer to these examples for illustrations of the commands that are described below.

The process analysis commands themselves are formatted according to a simple set of rules and a free-form format. Nevertheless, each command has a special syntax that must be followed, and each command makes use of special keywords and/or operators that have specific meaning to the

PACP. The commands are of three major types: global commands, IPR commands, and IRR commands. The discussion begins first, however, with a description of some general rules for entering the commands.

General Rules. The free-form format is similar to that used by the general mechanism processor. In general, white spaces are ignored, and line wrap around is allowed (i.e., commands can be continued on a subsequent line after a hard return). The free-form format also allows embedded comments and makes use of special symbols to indicate the type of input data. Special rules for naming species, entering labels, and specifying numerical values, such as stoichiometric coefficients and rate constant parameters, are also used. Each is discussed below:

- *Comments.* All lines that have an exclamation point in column 1 are treated as comment lines and are ignored by the PACP. Any text enclosed in braces ({}) or parentheses (()) is also treated as comment and ignored by the PACP.
- *Species names.* The PACP recognizes two types of species names: model species and user-defined Process Analysis species. “Model species” refer to species names in the Species Tables. (See the first part of this appendix.) These names must be spelled exactly as they appear in that table. The following special rules have been established for user-defined species names.
 - a) The Process Analysis species names must not contain any blanks and can be up to 16 characters long.
 - b) The name must begin with an alphabetic character but may contain any alphanumeric character (i.e., "A-Z", "a-z", and "0-9") or the characters ":" and "_" after the first position.
 - c) The name is case sensitive. Thus, NO2 and no2 would represent two different species.
 - d) A name can have embedded comments but cannot span two lines.
- *Label names.* For some of the IRR commands, reaction labels appearing in the chemical mechanism reaction list input file can be referenced. These labels would normally be spelled exactly as they appear in the chemical mechanism reaction list input file, except embedded comments and their delimiters should be omitted. However, any embedded blanks in those label names should be omitted, and the label name should contain no more than 16 non-blank characters.
- *Numbers.* Numerical inputs in the command file can be either integer (e.g., 5), floating point (e.g., 5.0), or exponential (e.g., 5.0E+00). With the exponential format, the "E" may be either upper or lowercase; a positive exponent will be assumed if the sign of the exponent is missing.

- *Command Line Terminator.* Input command lines are terminated by a semicolon.

Process Analysis Commands. This section describes the individual process analysis commands that are used to construct a PACP command file. In the description of these commands, the following conventions will be used. Bold type is used for PACP keywords and normal type for user supplied inputs. Alternative inputs are separated by vertical bars (|), and optional inputs are enclosed in braces ({}). The commands are as follows:

- *Process Analysis Global Commands.* The three process analysis global commands are shown in Table M-10. Each is discussed below:

OUTPUT_DOMAIN. As described above, Process Analysis outputs consist of IPRs and/or IRRs. These outputs are generated for the same time periods as the standard model-predicted concentrations. Like the concentration outputs, the Process Analysis outputs will be generated for every model grid by default unless this command is used to limit the Process Analysis output domain. Only one output domain can be specified, and it must be a block of contiguous cells. Although this command can appear anywhere in the input file, it is recommended that it be inserted near the beginning of the file. If the command occurs more than one time in the input file, the last entry will be used.

DEFINE FAMILY. This command is used to define a new species that can be referenced in other Process Analysis commands. The new species is limited to a linear combination of model species names (i.e., a family definition cannot reference another family). Families must be defined before they are referenced in other commands.

ENDPA. This command signifies the end of the PACP commands and thus should be the last command in the file.

- *Integrated Process Rate Command.* There is only one command for IPRs, and it controls the specific IPRs that are output. Its syntax and description is shown in Table M-11. Note that one command can cause many IPR outputs to be generated. For example, if one species or family is specified in a command but no process codes are specified, then one IPR will be generated for each science process for that species (i.e., 12 IPRs will be output). Similarly if the keyword ALL is used for the species name and no process code is specified, 12 IPRs will be generated for every model species. This would generate an output file that would be approximately 12 times as large as the corresponding concentration file! Also the impact on the CCTM memory requirements would be substantial, since adding a single IPR output has roughly the same effect as adding a model species. Thus, some caution should be exercised when formulating the commands to request IPR outputs.

The IPR outputs are written to an I/O API output file in exactly the same format and with the same number of time steps as the concentration output file. Since the I/O API currently has a limit of 120 output variables on a file, multiple files will be output if this limit is exceeded.

- *Integrated Reaction Rate Commands.* There are two types of IRR commands—global and output—and these are shown in Table M-12 and Table M-13, respectively. Each is discussed further below:

IRR_TYPE. This command controls the form of the IRR output that is generated. If it is omitted, then it will be assumed that a partial IRR analysis has been requested (i.e., IRR output commands are expected in the file.) If it is included, it should be inserted at the very beginning of the PACP command file. Note IRR type equal to full will cause one IRR to be generated for each chemical reaction in the gas-phase mechanism. If the I/O API limit of 120 variables per output file is exceeded, multiple output files will be generated.

DEFINE CYCLE. As noted in Table M-12, this command computes the net of the production and loss of a species, and assigns that value to a cycle name that can be referenced in the IRR output command. The command must appear before the cycle name is referenced. This command is useful when the same cycle is needed for multiple IRR outputs.

DEFINE RXNSUM. This command is similar to the cycle command, except that it allows the user to construct any linear combination of IRRs for individual chemical reactions. Again, this command is most useful when the same combination of IRRs is needed for multiple IRR outputs. The RXNSUM definition must precede any references to it in the command file.

IRR_OUTPUT. This is the command that causes a specific IRR output to be generated. As noted in Table M-13, the command can include a reference to a previously defined cycle or reaction sum name, a chemical reaction label, or one of the special operators that are described in Table M-14. One output variable is generated for each IRR_OUTPUT command. Since the operators can be fairly complicated, you are encouraged to review the Process Analysis output report whenever the IRR_OUTPUT command is used to ensure that the requested outputs are actually what you want. You are also referred to *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System* [Byun, D., and J.K.S. Ching, 1999] for a more detailed discussion of the operators and their use.

DESCRIPTION. This command allows you to provide a long description of the output variable. This description will be assigned to the long variable name on the I/O API output file.

Table M-10. Process Analysis Global Commands

OUTPUT_DOMAIN = {LOCOL[n₁] + HICOL[n₂] + LOROW[n₃] + HIROW[n₄] + LOLEV[n₅] + HILEV[n₆]};

The OUTPUT_DOMAIN command provides the capability to limit the IPR and IRR output data to a portion of the modeling domain. The n_i in brackets are numbers that define the bounds of the output domain relative to the number of columns, rows, and vertical levels in the modeling domain. Thus, for example, the value for n₁ must be greater than or equal to one and less than or equal to the number of columns in the domain. If any one domain specifier is omitted, the corresponding end of the modeling domain is used as a default. If the command is omitted entirely, output is generated for the entire domain.

DEFINE FAMILY familyname = {c₁*}species₁ {+ {c₂*}species₂ + ...};

The DEFINE FAMILY command is used to define a group of species as members of a family. The user specified "familyname" must be unique, and can be referenced in subsequent commands. The c_i are numerical coefficients that default to one if not specified; "species_i" represents the model species names.

ENDPA;

The ENDPA command signifies the end of the command input in the PACP command file.

Table M-11. Integrated Process Rate Output Command

IPR_OUTPUT species|familyname|**ALL** = {PCODE₁ + PCODE₂ + ...};

The IPR_OUTPUT command defines specific IPR outputs to be generated during a CMAQ CTM simulation. A model species name, family name, or the keyword ALL must follow the IRR_OUTPUT keyword. The keyword ALL refers to all model species. IPRs are generated for the selected species or family, and they are controlled by the specified values of PCODE_i, where PCODE_i corresponds to one of the process codes listed below. If no process codes are specified, IPRs will be generated for every science process (i.e., the first 12 codes shown below). The output variables that are generated are named either species_PCODE_i or familyname_PCODE_i.

Process codes and definitions:

XADV	Advection in the E-W direction
YADV	Advection in the N-S direction
ZADV	Vertical advection
ADJC	Mass adjustment
HDIF	Horizontal diffusion
VDIF	Vertical diffusion
EMIS	Emissions
DDEP	Dry deposition
CHEM	Chemistry
AERO	Aerosols
CLDS	Cloud processes and aqueous chemistry
PING	Plume-in-grid
XYADV	Sum of XADV and YADV
XYZADV	Sum of XADV, YADV, ZADV
TOTADV	Sum of XADV, YADV, ZADV, and ADJC
TOTDIF	Sum of HDIF and VDIF
VDIF	Sum of XADV, YADV, ZADV, ADJC, HDIF, and
TOTTRAN	

Table M-12. Integrated Reaction Rate Global Commands

IRR_TYPE = FULL|PARTIAL|NONE;

The IRR_TYPE command defines the type of IRR analysis. With the type set to FULL, IRRs for each individual reaction will be calculated and written to the IRR output file, and all other IRR commands will be ignored. IRR_TYPE set to PARTIAL indicates that the IRR commands following this command are to be processed to produce user-defined IRR outputs. Type set to NONE causes all IRR commands to be ignored and no IRR output to be generated. If the command is omitted, type PARTIAL is assumed.

DEFINE CYCLE cyclename = species₁;

The DEFINE CYCLE command is used to compute the net of all chemical production and loss of a species. Thus, this quantity is computed by summing the IRRs for all reactions in which a species is consumed, and then subtracting that sum from the sum of the IRRs for all reactions in which the species is produced. The "cyclename" is a user-defined name that must be unique, and can be referenced in subsequent IRR_OUTPUT commands.

DEFINE RXNSUM sumname = {c₁*}<rxlabel₁> { ± {c₂*} <rxlabel₂> ± ...};

The RXSUM command is used to compute a linear combination of the IRRs for individual reactions that can then be referenced in a subsequent IRR_OUTPUT command; "sumname" is user-defined and must be unique. The linear combination of IRRs is defined according to the expressions following the equal signs that specify which reaction's IRRs to sum. The "rxlabel_i" is the reaction label that is used in the generalized mechanism. The "c_i" are optional numerical coefficients that default to one if not specified.

Table M-13. Integrated Reaction Rate Output Commands

IRR_OUTPUT irrname = { c_1^* }op₁|cyclname{qual₁}|sumname{qual₁}|<rxlabl₁>
{ ± { c_2^* }op₂|cyclname{qual₂}|sumname{qual₂}|<rxlabl₂> + ...};

The IRR_OUTPUT command defines a specific IRR output to be generated during a CMAQ simulation. It is constructed by specifying a linear combination of IRR operators, IRR global definitions, or IRRs for specified reactions. Each individual term in the combination must include either one of the five IRR operators described in Table M-14 (i.e., op_i), a cycle name, a reaction sum name, or a reaction label enclosed in "greater than" and "less than" signs. The optional qualifiers (qual_i) for cyclename or reaction sum name can be either POSONLY or NEGONLY. With these qualifiers, the defined quantity is included as a term only when it is positive or negative, respectively. If the name is not qualified, the quantity is included regardless of sign. The numerical coefficients for each term (c_i) are assumed to be one unless they are explicitly included. The irrname that is supplied by the user will be assigned as the variable name in the I/O API IRR output file.

DESCRIPTION = 'description';

The description command is provided to allow the user to specify a long description of the output variable that will be included on the I/O API IRR output name. If a description is not specified for an IRR_OUTPUT variable, the irrname (or short name) will be used in the output file. If the description command is used, it should be located immediately following the IRR_OUTPUT command to which it applies.

Table M-14. Integrated Reaction Rate Output Operators

PROD[species₁] {FROM[species₂] {AND|OR [species₃] }}

The PROD operator is used to compute the total production of a species by summing the IRRs of all reactions in which species₁ appears as a product. The optional qualifiers FROM and/OR restrict the sum to include only those reactions in which species₂ and/or species₃ are reactants. The "species_i" can be any gas-phase mechanism species or a family of gas-phase species; "species₂" or species₃" may also be the keyword HV to restrict the selection to photolytic reactions.

NETP[species₁] {FROM[species₂] {AND|OR [species₃] }}

The NETP operator is very similar to the production operator since it is used to compute the production of a species. Whereas the PROD operator includes every reaction in which species₁ occurs as a product, the NETP operator includes only those reactions in which the net production of species₁ is greater than zero. Thus, if species₁ or any member of the family species appears as both a reactant and a product with equal stoichiometry in a reaction, the PROD operator will include it, but the NETP operator will not. This operator is useful for getting the net production of a family, for example.

LOSS[species₁] {AND|OR [species₂] }

The LOSS operator is used to compute the total loss of a species by summing the IRRs of all reactions in which species₁ appears as a reactant. The optional qualifier AND restricts the sum to include only those reactions in which both species₁ and species₂ are reactants. Similarly, the OR qualifier includes all reactions in which either "species₁" or "species₂" appears as a reactant, where "species₁" or "species₂" can be any gas-phase species in the mechanism, a family name that includes only gas-phase mechanism species, or the keyword HV to restrict the selection of reactions to those that are photolytic.

NETL[species₁] {AND|OR [species₂] }}

The NETL operator is very similar to the LOSS operator since it is used to compute the loss of a species. However, it includes only those reactions in which there is a net loss of "species₁" and/or "species₂". Thus, if species₁ or any member of the family species appears as both a reactant and a product with equal stoichiometry in reaction, the NETL operator will not include it in summing the loss of that species, whereas the LOSS operator will include the IRR for that reaction.

NET[species₁]

The NET operator is similar to the CYCLE definition since it gives the net of the production and the loss of a species for all reactions in which "species₁" appears either as reactant or a product; "species₁" may be any gas-phase, mechanism species or any family consisting wholly of gas-phase mechanism species.

Example M-3. Process Analysis Control Program Input Command File (PA_INPUT)

```
FAMILY OX = O3 + NO2 + 2*NO3 + O3P + O1D + PAN + HNO4  
+3*N2O5 + TPAN + OLN;
```

```
IRR_OUTPUT OXprod = NETP[OX];
```

```
DESCRIPTION = 'OX Production';
```

```
IRR_OUTPUT Oxloss = NETL[OX];
```

```
DESCRIPTION = 'OX Loss';
```

```
=====
! IRR_OUTPUT EXAMPLE 3 -- new OH
=====
```

```
DEFINE FAMILY VOCA = OL2 + OLI + OLT + ISO;
```

```
DEFINE CYCLE HONOcyc = H IRRTYPE = PARTIAL;
```

```
OUTPUT_DOMAIN = LOLEV[1] + HILEV[5];
```

```
=====
! IRR_OUTPUT EXAMPLES 1 and 2 -- OX Production & Loss
=====
```

```
DEFINE ONO;
```

```
DEFINE RXNSUM H2O2_OHcyc = <9> - <12> - <13>;
```

```
DEFINE RXNSUM HNO3_OHcyc = <P5> - <24>;
```

```
DEFINE RXNSUM OP1_OHcyc = <P13> - <88>;
```

```
DEFINE RXNSUM OP2_OHcyc = <P14> - <89> - <90> - <91> - <92> -  
<93> - <94> - <95> - <96> - <97> -  
<98> - <99> - <100> - <101>;
```

```
DEFINE RXNSUM PAA_OHcyc = <15> - <97>;
```

```
IRR_OUTPUT newOH = PROD [HO] FROM [O3] AND [VOCA] +  
2*H2O2_OHcyc[POSONLY] +  
HNO3_OHcyc[POSONLY] + HONOcyc[NEGONLY] +  
OP1_OHcyc[POSONLY] + OP2_OHcyc[POSONLY] +  
PAA_OHcyc[POSONLY];
```

DESCRIPTION = 'new OH';

!=====

! IRR_OUTPUT EXAMPLE 4 -- NO2 from HO2

!=====

IRR_OUTPUT NO2fromHO2 = PROD[NO2] FROM [HO2];

DESCRIPTION = 'NO2 FROM HO2';

!=====

! IRR_OUTPUT EXAMPLE 5 -- Net ONIT Production

!=====

IRR_OUTPUT netONIT = NET[ONIT];

DESCRIPTION = 'Net production of ONIT';

!=====

! IRR_OUTPUT EXAMPLE 6 -- OH reacting with VOC

!=====

DEFINE FAMILY VOC = {CH4 +} CO + ETH +HC3 + HC5 + HC8 + OL2 + OLT +
OLI + ISO + TOL + CSL + XYL + HCHO + ALD + KET +
GLY + MGLY + DCB;

IRR_OUTPUT lossOH_HC = LOSS[VOC] AND [HO];

DESCRIPTION = 'Loss of HC plus OH';

!=====

! IPR_OUTPUT EXAMPLES

!=====

IPR_OUTPUT NO;

IPR_OUTPUT VOC;

IPR_OUTPUT HCHO = CHEM + EMIS;

ENDPA;

IPR_OUTPUT(13) = XADV of VOC
IPR_OUTPUT(14) = YADV of VOC
IPR_OUTPUT(15) = ZADV of VOC
IPR_OUTPUT(16) = ADJC of VOC
IPR_OUTPUT(17) = HDIF of VOC
IPR_OUTPUT(18) = VDIF of VOC
IPR_OUTPUT(19) = EMIS of VOC
IPR_OUTPUT(20) = DDEP of VOC
IPR_OUTPUT(21) = CLDS of VOC
IPR_OUTPUT(22) = CHEM of VOC
IPR_OUTPUT(23) = AERO of VOC
IPR_OUTPUT(24) = PING of VOC
IPR_OUTPUT(25) = CHEM of HCHO
IPR_OUTPUT(26) = EMIS of HCHO

C INTEGRATED REACTION RATE SECTION

- c The following section gives a symbolic representation of how the
- c PARTIAL IRR outputs are calculated given the commands that were
- c included in the command file. The report includes pseudocode showing
- c how individual integrated reactions rates are combined to produce the
- c requested output. In the pseudocode that follows

C

- c $\text{IRR} < x >$ = the integrated reaction rate for
- c the reaction with label x as
- c defined in the chemical mechanism

C

c IRROUT(n) = the nth integrated reaction rate
c output that was requested

C

c Summary of Input IRR Commands for OUTPUT 1: OXprod

C

c The IRR_OUTPUT command was specified as follows:

C

c IRROUT(1) = NETP [OX]

C

6

c The referenced families are defined as follows:

C

```

c OX=O3+NO2+2*NO3+O3P+O1D+PAN+HNO4+3*N2O5+TPAN+OLN
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The referenced operators are defined as follows:
c
c..Net production of OX
c   Nprd( 1) =
c   & +     IRR< P5>! HNO3+hv=HO+NO2
c   & +     IRR< P21>! ONIT+hv=.2*ALD+.8*KET+HO2+NO2
c   & +     IRR< 9>! HO2+NO=NO2+HO
c   & + 2.0000 * IRR< 16>! NO+NO+O2=2*NO2
c   & + 2.0000 * IRR< 25>! HO+HNO3=NO3
c   & +     IRR< 50>! PAN+HO=HCHO+NO3+XO2
c   & +     IRR< 51>! ONIT+HO=HC3P+NO2
c   & +     IRR< 57>! MO2+NO=HCHO+HO2+NO2
c   & + 0.9640 * IRR< 58>! HC3P+NO=.75*ALD+.25*KET+.09*HCHO
c           ! +.036*ONIT+.964*NO2+.964*HO2
c   & + 0.9200 * IRR< 60>! HC5P+NO=.38*ALD+.69*KET+.08*ONIT+.92*NO2
c           ! +.92*HO2
c   & + 0.7600 * IRR< 62>! HC8P+NO=.35*ALD+1.06*KET+.04*HCHO
c           ! +.24*ONIT+.76*NO2+.76*HO2
c   & +     IRR< 64>! OL2P+NO=1.6*HCHO+HO2+NO2+.2*ALD
c   & +     IRR< 65>! OLTP+NO=ALD+HCHO+HO2+NO2
c   & +     IRR< 66>! OLIP+NO=HO2+1.45*ALD+.28*HCHO+.1*KET+NO2
c   & +     IRR< 67>! ACO3+NO=MO2+NO2
c   & +     IRR< 68>! TCO3+NO=NO2+.92*HO2+.89*GLY+.11*MGLY
c           ! +.05*ACO3+.95*CO+2*XO2
c   & +     IRR< 69>! TOLP+NO=NO2+HO2+.17*MGLY+.16*GLY+.7*DCB
c   & +     IRR< 70>! XYLP+NO=NO2+HO2+.45*MGLY+.806*DCB
c   & +     IRR< 71>! ETP+NO=ALD+HO2+NO2
c   & +     IRR< 72>! KETP+NO=MGLY+NO2+HO2
c   & +     IRR< 73>! OLN+NO=HCHO+ALD+2*NO2
c   & +     IRR< 131>! XO2+NO=NO2
c   & + 0.9120 * IRR< IS2>! ISO_RO+NO=.088*ONIT+.912*NO2+.912*HO2
c           ! +.912*ISOPRO+.629*HCHO
c   & + 1.2000 * IRR< IS9>! ISON_R+NO=NO2+.8*ALD+.8*ONIT+.8*HO2
c           ! +.2*ISOPRO+.2*NO2
c   & +     IRR<IS14>! IP_RO2+NO=NO2+HO2+.59*CO+.55*ALD+.25*HCH
c           ! +.08*GLY+.34*MGLY+.63*KET
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Pseudocode for OUTPUT 1: OXprod
cccccccccccccccccccccccccccccccccccccccccccccccccccccccc
  IRROUT( 1)=      Nprd( 1)

```



```

c & + IRR< 132> ! XNO2+NO2=ONIT
c & + IRR< IS6> ! ISO+O3=.6*HCHO+.65*ISOPRO+.39*ORA1+.27*H
c           !   +.07*HO2+.07*CO+.2*XO2+.2*ACO3
c           !   +.15*ALD
c & + IRR< IS7> ! ISO+O3P=.75*ISOPRO+.25*ACO3+.25*HCHO
c           !   +.25*MO2
c & + 2.0000 * IRR< IS8> ! ISO+NO3=ISON_R
c & + IRR<IS18> ! ISOPRO+O3=.268*HO+.1*HO2+.114*ACO3
c           !   +.054*MO2+.07*XO2+.155*CO+.146*HCHO
c           !   +.02*ALD+.01*GLY+.85*MGLY+.09*KET
c           !   +.462*ORA1
c & + 2.0000 * IRR<IS20> ! ISOPRO+NO3=.075*ACO3+.075*HNO3+.643*CO
c           !   +.282*HCHO+.925*ONIT+.282*ALD
c           !   +.925*HO2+.925*XO2
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Pseudocode for OUTPUT 2: Oxloss
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
IRROUT( 2) =      NLOS( 1)

```

```

cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Summary of Input IRR Commands for OUTPUT 3: newOH
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The IRR_OUTPUT command was specified as follows:
c
c IRROUT( 3) =      PROD [HO] FROM [O3] AND [VOCA]
c &      + 2.0000 * H2O2_OHcyc[POSONLY]
c &      +      HNO3_OHcyc[POSONLY]
c &      +      HONOcyc[NEGONLY]
c &      +      OP1_OHcyc[POSONLY]
c &      +      OP2_OHcyc[POSONLY]
c &      +      PAA_OHcyc[POSONLY]
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The referenced families are defined as follows:
c
c VOCA=OL2+OLI+OLT+ISO
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The referenced cycles are defined as follows:
c

```

```

c..CYCLE 1 HONOcyc
c   CYSM( 1) =
c   & -      IRR< P4>! HONO+hv=HO+NO
c   & +      IRR< 15>! NO+HO=HONO
c
c   ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c   c The referenced reaction sums are defined as follows:
c
c..RXSUM 1 H2O2_OHcyc
c   RXSM( 1) =
c   & +      IRR< 9>! HO2+NO=NO2+HO
c   & -      IRR< 12>! HO2+HO2=H2O2
c   & -      IRR< 13>! HO2+HO2+H2O=H2O2
c
c..RXSUM 2 HNO3_OHcyc
c   RXSM( 2) =
c   & +      IRR< P5>! HNO3+hv=HO+NO2
c   & -      IRR< 24>! HO+NO2=HNO3
c
c..RXSUM 3 OP1_OHcyc
c   RXSM( 3) =
c   & +      IRR< P13>! OP1+hv=HCHO+HO2+HO
c   & -      IRR< 88>! HO2+MO2=OP1
c
c..RXSUM 4 OP2_OHcyc
c   RXSM( 4) =
c   & +      IRR< P14>! OP2+hv=ALD+HO2+HO
c   & -      IRR< 89>! HO2+ETHP=OP2
c   & -      IRR< 90>! HO2+HC3P=OP2
c   & -      IRR< 91>! HO2+HC5P=OP2
c   & -      IRR< 92>! HO2+HC8P=OP2
c   & -      IRR< 93>! HO2+OL2P=OP2
c   & -      IRR< 94>! HO2+OLTP=OP2
c   & -      IRR< 95>! HO2+OLIP=OP2
c   & -      IRR< 96>! HO2+KETP=OP2
c   & -      IRR< 97>! HO2+ACO3=PAA
c   & -      IRR< 98>! HO2+TOLP=OP2
c   & -      IRR< 99>! HO2+XYLP=OP2
c   & -      IRR< 100>! HO2+TCO3=OP2
c   & -      IRR< 101>! HO2+OLN=ONIT
c
c..RXSUM 5 PAA_OHcyc
c   RXSM( 5) =
c   & +      IRR< 15>! NO+HO=HONO

```

```

c & -      IRR< 97>! HO2+ACO3=PAA
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The referenced operators are defined as follows:
c
c..Production of HO from O3 and VOCA
c   PROD( 1)=
c   & + 0.1000 * IRR< 85>! OLT+O3=.53*HCHO+.5*ALD+.33*CO+.2*ORA1
c           ! +.2*ORA2+.23*HO2+.22*MO2+.1*HO
c   & + 0.1400 * IRR< 86>! OLI+O3=.18*HCHO+.72*ALD+.1*KET+.23*CO
c           ! +.06*ORA1+.29*ORA2+.26*HO2+.14*HO
c           ! +.31*MO2+OLIAER
c   & + 0.2700 * IRR< IS6>! ISO+O3=.6*HCHO+.65*ISOPRO+.39*ORA1+.27*H
c           ! +.07*HO2+.07*CO+.2*XO2+.2*ACO3
c           ! +.15*ALD
c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Pseudocode for OUTPUT 3: newOH
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
    IRROUT( 3)= 0.0

IF( RXSM( 1) .GT. 0.0 ) THEN
    IRROUT( 3)= IRROUT( 3) + 2.0000 * RXSM( 1)
ENDIF

IF( RXSM( 2) .GT. 0.0 ) THEN
    IRROUT( 3)= IRROUT( 3) + RXSM( 2)
ENDIF

IF( CYSM( 1) .LT. 0.0 ) THEN
    IRROUT( 3)= IRROUT( 3) + ABS(CYSM( 1))
ENDIF

IF( RXSM( 3) .GT. 0.0 ) THEN
    IRROUT( 3)= IRROUT( 3) + RXSM( 3)
ENDIF

IF( RXSM( 4) .GT. 0.0 ) THEN
    IRROUT( 3)= IRROUT( 3) + RXSM( 4)
ENDIF

IF( RXSM( 5) .GT. 0.0 ) THEN
    IRROUT( 3)= IRROUT( 3) + RXSM( 5)
ENDIF

```

IRROUT(3) = IRROUT(3)
& + PROD(1)

cc
c Summary of Input IRR Commands for OUTPUT 4: NO2fromHO2
cc
c
c The IRR_OUTPUT command was specified as follows:
c
c IRROUT(4) = PROD [NO2] FROM [HO2]
c
cc
c
c The referenced operators are defined as follows:
c
c..Production of NO2 from HO2
c PROD(1)=
c & + IRR< 9> ! HO2+NO=NO2+HO
c
cc
c Pseudocode for OUTPUT 4: NO2fromHO2
cc
IRROUT(4) = PROD(1)

cc
c Summary of Input IRR Commands for OUTPUT 5: netONIT
cc
c
c The IRR_OUTPUT command was specified as follows:
c
c IRROUT(5) = NET [ONIT]
c
cc
c
c The referenced operators are defined as follows:
c
c..Net reaction of ONIT
c NETR(1)=
c & - IRR< P21> ! ONIT+hv=.2*ALD+.8*KET+HO2+NO2
c & - IRR< 51> ! ONIT+HO=HC3P+NO2
c & + 0.0360 * IRR< 58> ! HC3P+NO=.75*ALD+.25*KET+.09*HCHO
c ! +.036*ONIT+.964*NO2+.964*HO2
c & + 0.0800 * IRR< 60> ! HC5P+NO=.38*ALD+.69*KET+.08*ONIT+.92*NO2
c ! +.92*HO2

```

c & + 0.2400 * IRR< 62> ! HC8P+NO=.35*ALD+1.06*KET+.04*HCHO
c           !   .24*ONIT+.76*NO2+.76*HO2
c & +     IRR< 101> ! HO2+OLN=ONIT
c & +     IRR< 132> ! XNO2+NO2=ONIT
c & + 0.0880 * IRR< IS2> ! ISO_RO+NO=.088*ONIT+.912*NO2+.912*HO2
c           !   .912*ISOPRO+.629*HCHO
c & + 0.8000 * IRR< IS9> ! ISON_R+NO=NO2+.8*ALD+.8*ONIT+.8*HO2
c           !   .2*ISOPRO+.2*NO2
c & +     IRR<IS10> ! ISON_R+HO2=ONIT
c & +     IRR<IS11> ! ISON_R+ACO3=.5*HO2+.5*MO2+.5*ORA2+ALD
c           !   +ONIT
c & +     IRR<IS12> ! ISON_R+MO2=.5*HCHO+.5*HO2+ALD+ONIT
c & + 0.9250 * IRR<IS20> ! ISOPRO+NO3=.075*ACO3+.075*HNO3+.643*CO
c           !   .282*HCHO+.925*ONIT+.282*ALD
c           !   .925*HO2+.925*XO2
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Pseudocode for OUTPUT 5: netONIT
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
IRROUT( 5) =      NETR( 1)

cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c Summary of Input IRR Commands for OUTPUT 6: lossOH_HC
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The IRR_OUTPUT command was specified as follows:
c
c   IRROUT( 6) =      LOSS [VOC] AND [HO]
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The referenced families are defined as follows:
c
c
VOC=CO+ETH+HC3+HC5+HC8+OL2+OLT+OLI+ISO+TOL+CSL+XYL+HCHO+ALD+KET

c     +GLY+MGLY+DCB
c
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c The referenced operators are defined as follows:
c
c..Loss of VOC and HO
c   LOSS( 1)=
c   & +     IRR< 29> ! CO+HO=HO2

```

***** END OF PROCESS ANALYSIS CONTROL PROGRAM OUTPUT REPORT