DEVELOPMENT OF AN IMPROVED EMISSIONS SPECIATION DATABASE FOR PROCESSING VOC EMISSIONS FOR AIR QUALITY MODELS

BACKGROUND

EMISSIONS PROCESSING IS THE MAJOR OBSTACLE TO IMPLEMENTING NEW OR DETAILED MECHANISMS INTO AIRSHED MODELS

ADDRESSING THIS HAS TWO COMPONENTS

- IMPROVING EMISSIONS PROCESSING AND CHEMISTRY IMPLEMENTATION SOFTWARE

- ASSIGNING SPECIES IN THE MECHANISM TO THE EMISSIONS SPECIATION CATEGORIES

PROBLEMS WITH CURRENT EMISSIONS SPECIATION DATABASES MAKE IT VERY DIFFICULT TO MAKE MECHANISM ASSIGNMENTS PROPERLY

- EPA, CALIFORNIA, TEXAS, PROBABLY OTHERS USE INCOMPATIBLE SPECIES CATEGORIZATIONS

- MANY CATEGORIES ARE REDUNDANT, POORLY-DEFINED OR REFER TO COMPLEX MIXTURES

- ASSIGNING MODEL SPECIES REQUIRES MAKING ASSUMPTIONS ABOUT WHAT THESE REFER TO

- THIS CAUSES INCONSISTENT OR INAPPROPRIATE MECHANISM ASSIGNMENTS

CURRENT MCNC-UCR PROJECT

OBJECTIVE

IMPLEMENT THE SAPRC-99 MECHANISM INTO THE SMOKE EMISSIONS PROCESSING SYSTEM

APPROACH

DEVELOP AN IMPROVED EMISSIONS SPECIATION DATABASE AND MAKE MECHANISM ASSIGNMENTS

DEVELOP SOFTWARE TO IMPLEMENT SPECIATION DATABASE AND ASSIGNMENTS IN SMOKE

TEST PROGRAMS AND DEMONSTRATE APPLICABILITY TO REACTIVITY ASSESSMENT

OPTIONALLY UPDATE SMOKE'S JAVA-BASED USER INTERFACE TO ASSIST IN REACTIVITY ASSESSMENT

CURRENT STATUS

CONTRACTS BETWEEN ACC AND MCNC AND MCNC AND UCR ABOUT TO BE SIGNED

SIGNIFICANT PROGRESS MADE ON THE SPECIATION DATABASE AND MECHANISM ASSIGNMENTS UNDER FUNDING FROM THE UNIVERSITY OF HOUSTON

SPECIATION DATABASE PROGRESS

CATEGORIES USED BY EPA, CALIFORNIA, TEXAS, SPECIATE 3.1 AND SAPRC-99 COMBINED INTO A SINGLE DATABASE

DUPLICATES REMOVED

EACH CATEGORIZED AS ONE OF FOLLOWING:

Cd	DESCRIPTION	NUMBER
1	SINGLE COMPOUND	1304
2	ISOMERIC MIXTURE	297
3	COMPLEX MIXTURE	185
4	POORLY DEFINED	32

ASSIGNMENTS FOR COMPOUNDS

NUMBERS OF EACH TYPE OF ATOM AND THE CORRESPONDING MOLECULAR WEIGHT

CAS ID NUMBERS IN ALL BUT A FEW CASES

MECHANISM ASSIGNMENTS MADE:	NUMBER
SAPRC-99 DETAILED	920
SAPRC-99 LUMPED	1181
CARBON BOND (PRELIMINARY)	1196
RADM 2 (NOT YET DONE)	0
NON-VOLATILE	43

SPECIATION DATABASE PROGRESS
(CONTINUED)

ASSIGNMENTS FOR MIXTURES

ALL ISOMERIC AND 78 COMPLEX MIXTURES ASSIGNED TO MIXTURES OF COMPOUNDS

33 COMPLEX MIXES ASSIGNED AS NON-VOLATILE

NO DIRECT MECHANISM ASSIGNMENTS MADE FOR ANY MIXTURES

EXTENT OF MASS OF EPA MODELS-3 TOTAL EMISSIONS PROFILES CURRENTLY ASSIGNED:

SAPRC-99 DETAILED MODEL SPECIES 93.4%
CONDENSED MECHANISM SPECIES..........98.9%

IMPLEMENTATION

IMPLEMENTED IN AN EXCEL SPREADSHEET

MACROS WRITTEN FOR FOLLOWING FUNCTIONS:

- COMPILE MECHANISM ASSIGNMENTS FOR MIXTURES USING THOSE FOR CONSTITUENTS

- CREATE MODEL SPECIES ASSIGNMENTS FOR EXISTING EMISSIONS CATEGORIES

- PROCESS SPECIFIC EMISSIONS PROFILES TO OBTAIN MODEL SPECIES COMPOSITIONS

DATABASE SPREADSHEET AND DOCUMENTATION AVAILABLE AT http://www.cert.ucr.edu/~carter/emitdb

REMAINING WORK

COMPLETE DOCUMENTATION OF DATABASE

UPDATE AND IMPROVE MECHANISM AND MIXTURE COMPOSITION ASSIGNMENTS WHERE POSSIBLE

MAKE ASSIGNMENTS FOR RADM-2 MECHANISM FOR USE WITH MODELS-3

IMPLEMENT CAPABILITY TO DERIVE EMISSIONS-DEPENDENT SAPRC MECHANISM PARAMETERS

IMPLEMENT DATABASE IN EMISSIONS PROCESSING SOFTWARE (OTHER TASKS ON MCNC PROJECT)

MAKE DATABASE MORE ACCESSIBLE AND EASIER TO USE AND UPDATE BY OTHERS

SUCCESS IN THIS PROJECT REQUIRES THAT THE DATABASE BE USED AND UPDATED IN FUTURE EMISSIONS AND MECHANISM DEVELOPMENT WORK

EXTERNAL INPUT AND PEER REVIEW NECESSARY FOR THIS TO OCCUR

CENTRAL CLEARING HOUSE NEEDED FOR SPECIATION PROFILES