The Emissions Inventory Maintenance Application

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ABSTRACT

The Air Quality Management Decision Support System (AQMDSS) is a comprehensive set of software tools that includes the complete data path from emission inventory development through emissions processing, air quality modeling, and data analysis. The AQMDSS uses the Multimedia Integrated Modeling System (MIMS) as the user interface for setting up and executing the Sparse Matrix Operator Kernel Emissions (SMOKE) processing system, the AMS/EPA Regulatory Model (AERMOD) and its AERMAP and AERMET preprocessors, the Models-3/Community Multiscale Air Quality (CMAQ), and other data preparation and analysis tools.

This paper is an update to one that was presented at the 14th Annual Emission Inventory Conference in Las Vegas, NV in 2005.¹ At that time, the design phase was complete and implementation was proceeding. The AQMDSS is now installed at the Beijing Municipal Environmental Protection Bureau (BMEPB) in Beijing, China.

First, this paper focuses on the Emissions Inventory Maintenance Application (EIMA) of the AQMDSS. Key features include a relational database implementation of an extended National Emission Inventory (NEI) Input Format (NIF) version 3; menu-driven, multilingual user interface that supports data integrity; security for user access of data; and direct access to data tables via Structured Query Language (SQL).

Next, this paper describes how the EIMA was implemented at the BMEPB. We will report our experience with performing bulk data loads into the NIF 3.0 data format using SQL.

INTRODUCTION

The Air Quality Management Decision Support System (AQMDSS) was built for the Beijing Municipal Environmental Protection Bureau (BMEPB) of Beijing Municipal Government (BMG) in the People's Republic of China. Figure 1 illustrates the schematic of the primary components in the completed system.²

Figure 1. Primary system schematic of the Air Quality Management Decision Support System. (From RTI International, "System Analysis and Design Report for the Air Quality Management Decision Support System – Revised Version," Prepared for PA Consulting Group by RTI International, Research Triangle Park, NC 2004.)



ExtractorsInserters

The AQMDSS was designed and implemented by RTI International as an integrated software system to support air quality modeling at multiple scales. The initial design was to integrate existing software – models and associated tools – into a common framework, which would provide users with a friendly, graphical user interface (GUI).³ Also, data would be entered and stored in a database, from which data files would be generated as needed by the models. No changes would be made to the models to ease upgrading as newer versions of models were released in the future.

When gathering the models and tools, however, we were not able to locate a publicly available application for building and maintaining the emissions inventory data. Instead of a readily available tool, we found that a wide variety of tools had been created by various organizations (e.g., States) over the years. BMEPB, however, needed a way to build a new emissions inventory and store it in the database. To fill this need we created the Emissions Inventory Maintenance Application (EIMA).

The next section discusses the main features of the EIMA. Then, we present our experience with installing the EIMA on the computer system in Beijing and performing bulk data loads into the database. At the end we present our conclusions.

MAIN FEATURES OF THE EIMA

System requirements of the AQMDSS impacted the design and implementation of the EIMA. These included a user interface in both Simplified Chinese and English, data access limited to authorized users, and data integrity for processing the data with the Sparse Matrix Operator Kernel Emissions (SMOKE) processing system. It also needed to support the parent/child relationships among data tables in the database, while being flexible to support future additions to the data structure. The remainder of this section discusses the main features of the EIMA.

Flexibility

The components of the AQMDSS are applications that are periodically updated. For example, SMOKE typically has at least one new release each year. To accommodate updates as quickly as possible, the AQMDSS and the EIMA must be extremely flexible.

Maximizing flexibility requires minimizing the changes required in the AQMDSS when one model is changed. To meet this need the AQMDSS was built using object-oriented design of reusable components. For example, if the data structure for one model input file is changed, then the only components that must be changed are the one extractor for that data file, the data elements in the database that support that data file, and the EIMA screens for those data elements.

User Interface

The BMEPB required the user interface to be in Simplified Chinese. Contractors and other consultants from outside China, however, primarily used English as their first language. An early requirement, therefore, was that the EIMA have a multilingual user interface.

The Java programming language includes support for internationalization/localization (i.e., i18n/l10n). This construct allows the text displayed by the program to be stored separately from the program itself. The EIMA was constructed using this construct, so text such as the titles of frames and the descriptions of input fields are stored in text files.

Currently, the EIMA is distributed with 2 sets of these files – English and Simplified Chinese. The language that is displayed is determined by the user's environment, as defined for his user ID in the operating system. English is the default language, so if the user ID is set up for Simplified Chinese then that is how the screens are displayed, otherwise English is used. To support another language, such as Spanish, a new set of text files need to be created for that language. The screens would then be displayed in that new language for any user ID that uses it. No changes are required for the program itself, and only one version of the program must be maintained.

Types of Users

The AQMDSS supports many different types of users. Each type of user performs a specific job function. For example, some users may analyze model results and create visualizations but may not execute models. These users would need access to only the visualization tools and model output files. Similarly, a user who works with AERMOD for industrial-scale modeling would not need access to SMOKE.

The structure of EIMA also supports users by type. Each user ID authorized for access to the AQMDSS is assigned a user type. The most restricted user type performs only visualization work, while the most expert type has access to all functions of the entire AQMDSS. Some of these users also need access to the EIMA. So, a user ID designated as *area source modeler* has access to data entry and update screens for data tables related to area sources, but cannot enter data for point sources.

The EIMA menu for each user is constructed such that only the parts of the system for which he/she has access are shown. Other parts cannot be accessed through the EIMA screens. This is the first level of data security. Figure 2 shows the data maintenance screen for an *expert* user.

Data Maintenance		_ . .			
Select Table to Modify From a Table Group		<u> </u>			
Table Groups Table Description					
Scenario Data Meteorological Scenarios 👻	Add	Update			
Area Source Data Area Source Processes 🗸 🗸	Add	Update			
On-Road Mobile Source Data Reference Counties for On-Road Mobile Sources 🗾	Add	Update			
Biogenic Source Data BEIS3 Emission Factors 👻	Add	Update			
Point Source Data Sites for Point Sources					
Growth and Control Data ALLOWABLE Control Packet - Add Update					
Ambient Data Ambient Stations Add Update					
AERMOD Data AERMOD Site Data 👻					
Gridded Results Gridded Results 🗸					
Supporting Tables Ambient Data Parameters	Add	Update			
Master Tables Types of Point Releases 🗸	Add	Update			
Done		•			

Figure 2. Data maintenance screen for user type expert.

Data Security

Security must be set up very carefully. Each user must be allowed access to the parts of the AQMDSS that are appropriate to their job functions, but not to other parts. Three levels of security are provided with the AQMDSS, as follows.

- The operating system is responsible for validating that the user has access to the computer system. This is accomplished via user ID/password. When a systems administrator creates an account for a user, he/she also places the user into one or more groups and defines the parts of the system to which that user has access. The operating system then grants access to directories, files, and programs based on the permissions for that user ID.
- The EIMA is responsible for validating that the user has access to that application. This is accomplished via user ID and password for the underlying database of the AQMDSS. An expert user defines each user in the database and assigns a user type. The EIMA constructs the data maintenance menu for each user based on his assigned type.
- PostgreSQL is responsible for validating the user's access to the database and individual data tables. An expert user (i.e., a database administrator) creates a user account for the database and assigns the user to one or more database groups. PostgreSQL has a list of permissions which may be granted for each table in a database, and the database administrator defines which permissions are to be given to each user or group. PostgreSQL then allows or blocks the various types of access to its tables.

The person responsible for maintaining database security needs to grant permissions consistently for the EIMA and for PostgreSQL. For example, a new user may be assigned user type *area source modeler*, so the EIMA gives that user access to enter data into area source-related data tables. But, if that user is not also granted permission within PostgreSQL to all of those data tables, then PostgreSQL will block some or all of that user's activities with respect to some tables.

Data Entry and Validation

The data structure of an emission inventory is very complex. Many items are represented by numeric or alphanumeric codes (e.g., pollutant code, facility ID). Certain codes may appear to be numeric, but cannot be stored that way because some valid data values have a leading zero (e.g., state and county FIPS codes). Other fields must contain only certain valid values (e.g., less than or equal to seven days per week). These types of data validation are set up within the EIMA, so restricted data values are validated when they are entered.

For some data, the information's structure is too complex to exist in one data table; it is split into related tables. A good example of this is a point source. One facility is a point source, but it may have multiple processes, with multiple emission points, control equipment, and pollutants. The NIF v3.0 data format handles this situation by dividing the data elements for one point source into data records residing in multiple, related data tables using a relational design.

The AQMDSS database encompasses the NIF v3.0 relational design and implements it in PostgreSQL. Relationships between tables are explicitly defined in the data structure using primary keys, foreign keys, and unique keys. Returning to the example of a point source, the keys defined in its tables form parent/child relationships. The facility is the parent of processes (i.e., a process is a child of the facility) and must have a record in the appropriate data table before any processes can be entered for that facility.

The EIMA supports the NIF-3 structure. A user cannot directly enter data for a child table. Instead, the record in the parent table must first be created, completed, and saved; then data can be entered for a child table. Also, data in fields that identify a record in the database, such as a facility ID, cannot be changed after committing the record to the database. This feature prevents orphaned records (i.e., a child record whose link to its parent record is broken)

User Notes

The emission inventory can be expected to frequently change. For example, errors from the past may be found and corrected, control equipment for a source may be changed, or emission factors may be updated. The EIMA includes a feature that enables the user to document these changes when making them.

Each data entry screen includes a button for the user to enter a free-form note. When a value is changed, the user may want to record the old value, the reason for the change, and the source of the new value. By keying this information into a note that is stored in the database and attached to the specific data record, this type of information can be captured. The EIMA automatically records the ID of the user who created the note and the date and time of the entry, allowing a series of notes to be associated with any data record.

SET UP AT BMEPB

Set up of the AQMDSS and specifically the EIMA at Beijing Municipal Environmental Protection Bureau in Beijing was done by a team consisting of two RTI team members, the Beijing Technical Expert and numerous BMEPB employees. All together a group of roughly 10 people worked on the system at one point or another during the week long setup. Many of the people involved had an interest in a particular component of the system (e.g., GIS) and participated only in the part they would eventually use.

BMEPB had purchased 4 Pentium Dual-Processors 64 Bit Xenon rack-mount servers, 2.4 GHZ with HyperThreading. Each machine had 4 GB of RAM and a 200 GB SCSI hard drive. Extra drive space was available through a Samba mount, however it was not needed. Each machine was connected to a Gigabit switch. The Internet was not connected to the BMEPB computational machine.

Redhat AS 4 was installed by the Chinese expert upon arrival of the RTI team. All work on the machines was done using the Simple Chinese character set. X-Windows, PostgreSQL, and several Linux utilities were installed by the Redhat installation media and were not altered.

The climate controlled section of the lab held numerous servers including the ones used for this project. Some work was done standing at the console; however, the team usually sat at a console in the lab using VNC Viewer on a windows XP machine.

Java plays a crucial role in setting up the system. The client had wanted to use the SUN Hotspot java edition, but we found upon testing at the site that it was incompatible with MIMS. The reason for this was never determined. Instead, we used the SUN J2SE 64-bit version tested by RTI. Due to Linux's isolation of libraries, this required a simple change to the \$JAVA_HOME environment variable. Also simplified was the transition from 32-bit to 64-bit. We switched seamlessly between 32- and 64-bit for development and testing using the SUN JVM.

NIF3 Data Format

Examination of the NIF3 database format implemented by RTI shows that most tables have a dependency on one or more tables that must be filled before population can occur. These dependencies are enforced by the database structure and cannot be ignored when importing data.

Populating Data Tables for Point Sources

For example if a user had some point source emission data for SMOKE that they wanted to enter and later extract for the PTINV file, they would need to fill a series of tables that would ultimately uniquely identify each data point. Along the way they would identify such information as the location in space, the facility id, the source, and ultimately the pollutant.

The following pages go through an example of starting at the highest level table (state_county_fips_codes) filling dependencies before filling dependent tables. Several figures are included to illustrate the layout of the database as well as usage of the EIMA. All diagrams for the database are created by the SCHEMASpy documentation system (http://schemaspy.sourceforge.net/).

At the top level are the country_code, time_zones, and state_county_fips_code tables. Figure 3 shows the relationship between the top level tables.

Figure 3. The state_county_fips_codes table is the first step in identifying point source information.

	state_county_fips_codes		
	state_county_fips_code bpchar[5]		
	state_county_fips_code_desc	varchar[60]	
	state_fips_code	bpchar[2]	
code	county_fips_code	bpchar[3]	
country_code	date_created	timestamp[8]	
country_name	userid_created	varchar[20]	
date_created	date_modified	timestamp[8]	
userid_created	userid_modified	varchar[20]	
date_modified	★ country_code	bpchar[2]	
userid_modified	🗸 county_std_tz	bpchar[3]	
5 rows 8 >	dst_code	bool[1]	
/	county_pop	int4[4]	
time_zones	county_pop_yr	int4[4]	
tz_code	< 2 8,738 rows	68 >	
tz_desc			
22 rows 2 >			

When used together, these tables identify the area in which the facility is located. While this works wonderfully in the United States the RTI team found that it could be adapted to other organizational structures. For instance the Chinese use province/state organizations. Working in concert

with BMEPB we mapped the provinces to the state FIPS and district to the county FIPS. While slightly artificial it proved to be a good compromise for importing data.

Included in most tables are 4 fields: date_created, userid_created, date_modified, and userid_modified. These fields are used by the EIMA in conjunction with security to help identify who and when changes are made.

After filling the location tables, a series of facilities must be entered into the point_source_site table. Looking at the keys for the point_source_site table we see that it references state_county_fips. Therefore any data previously entered for the state_county_fips table will satisfy relevant dependencies for the point_source_site table, as illustrated in Figure 4.

Figure 4. Keys for the point_source_site table.

Indexes:	
Column(s)	Туре
country_code + state_county_fips + pt_facility_id	Primary key
pt_facility_id	Must be unique

Though not strictly required, each table has several pieces of supporting information to make the information in the database more useful. These fields often link into other tables to help narrow the scope of what can be entered into the database. For example, the facility_category_code links to the facility_category table. Thus any entries into that field must reside in the facility_category table. Additional fields are shown in Figure 5.

Figure 5. Supporting information in the point_source_site table.

	point_source_	site		
country_	code	bpchar[2]		
state_co	state_county_fips bpchar[5			
pt_facilit	y_id	varchar[15]		
facility_i	d_2	varchar[12]		
facility_c	ategory_code:	bpchar[2]		
cems_fa	icility_code	varchar[6]		
_sic_prim	ary	bpchar[4]		
facility_r	ame	varchar[80]		
site_de s	cription	varchar[40]		
location	address	varchar[50]		
city		varchar[60]		
county		varchar[40]		
province		varchar[40]		
postal_code		varchar[14]		
facility_la	atitude	float8[8]		
facility_longitude		float8[8]		
facility_elevation		float4[4]		
facility_location		point[16]		
tri_id varchar[20		varchar[20]		
date_created		timestamp[8]		
userid_created		varchar[20]		
date_modified		timestamp[8]		
userid_r	nodified	varchar[20]		
< 4	101 rows	7 >		

The EIMA requires that the user enter all required information before moving on to secondary fields. Looking at point_source_site table specifically we see in Figure 6 that the three required fields of country_id, fips, and facility_id are input first. Both country_id and fips are drop-down boxes so that the user can use only previously entered values (from the appropriate table).

Adding a Record (Part I: Primary Fields) - • × Enter or Select Primary Values to Create a New Record ۰ Table: Sites for Point Sources Variable Values Range Permitted Values Value Country ID No Range Show Values 0 Ŧ FIPS 0 No Range Show Values • Facility ID No Range ОK Done Add Note for This Record

Figure 6. Inputting required information into the EIMA.

When the user indicates completion, then the database checks each constraint to be sure it is a valid selection. If no errors are found, then the value is written to the database and the user is notified of a successful write as seen in Figure 7.



Figure 7. When valid data are entered, the data are written to the database.

A final window comes up with the rest of the fields in the table as seen in Figure 8. The Value Range and Permitted Values fields show any constraints that the database may impose on entered values. Value ranges might be something like 0-100 while Permitted Values will be types of data such as integers or characters.

_ 🗆 🗙 Adding a Record (Part II: Additional Fields) Enter or Select Additional Values to Create a New Record Table: Sites for Point Sources Variable Values Range Permitted Values Value Additional Facility ID No Range na Facility Category ID No Range 01 na Ŧ CEMS Facility ID No Range na SIC ID No Range 0 na Ŧ Name of Facility No Range na Site Description No Range na Address No Range na City No Range na County No Range na Province No Range na Doctol Cod

Figure 8. More data to be entered for point_source_site table.

Notice that field for facility_category_ID presents a drop down list that links to facility_category table. This ensures that only values in that table can be selected, forcing consistency throughout all records for this table.

After entering data for a facility in the point_source_site table, each emission unit may be added to the point_source_er table. As shown in Figure 9, the values for the country_code, state_county_fips, and pt_facility_id are carried along to the primary key of this table. The value of pt_eu_id is added to the primary key, allowing multiple emission units to be entered for each facility.

Figure 9. Keys for point_source_er.

Indexes:	
Column(s)	Туре
country_code + state_county_fips + pt_facility_id + pt_eu_id	Primary key

Looking at the table for point_source_er in Figure 10 we see that quite a few non-key dependencies have been added. Most tables in the database ultimately have many dependencies. Understanding these is the key to successfully entering data.

Figure 10. More linkages are added as needed to help fill tables.



However, a closer look at the table definition in Figure 11 shows that the only fields that cannot be null, in addition to those comprising the primary key, are sic_eu, user_id_created, and date_created. This means that we will have to go back and fill only the SIC table with each sic_eu we intend to use.

Figure 11. Table definition for point_source_er.

Column	Туре	Size	Nulls	Auto	Default	Children	Parents
country_code	bpchar	2					state county fips codes
state_county_fips	bpchar	5					state county fips codes
pt_facility_id	varchar	15					
pt_eu_id	varchar	6					
er_point_type	bpchar	2					<u>emission release point type</u>
cems_boiler_id	bpchar	5	\checkmark		null		
sic_eu	bpchar	4					sic
design_capacity	float4	4	\checkmark		null		
design_capacity_unit_numerator	varchar	10	$\overline{\mathbf{A}}$		null		<u>unit codes</u>
design_capacity_unit_denominator	varchar	10	\checkmark		null		unit codes
max nameplate capacity	float4	4	\sim		null		
eu_description	varchar	80	\checkmark		null		
stack_height	float4	4			null		
stack_diameter	float4	4	. √		null		
stack_fenceline_distance	float4	4	Ý		null		
exit_gas_temp	float4	4	Ý		null		
exit_gas_velocity	float4	4	Ý		null		
exit_gas_flow_rate	float8	8	Ą		null		
x_coordinate	float8	8	Ň		null		
y_coordinate	fioat8	8	N.		null		
xy_coordinate_type	varchar	8	Υ,		null		<u>xy coordinate type</u>
stack_elevation	float4	4	Ň		null		
er_location	point	16	N.		null		
nunzuntai_area_iugitive	IFILØ int0	0	۲ 		nuii		
fugitive upit	Warebar	10	ू र		nuii		upit codec
release at description	varchar	00	al a		nui		
herizoptal method code	bochar	00	4		nuii		barizantal collection mathed
horizontal_methou_code	uprobor	- C	, d		nun		nonzonial collection method
horizontal_accuracy	varchar	0 2	۲ م		nuii		barizantal reference datum anda
	bpchar	- -	, d		nui		nonzontal reference uatum code
	openar	J 40	, Y		nui		reference point code
source_map_scale_number	Varchar	10	۷ م		nuii		
	upunar tima atawa a	О	γ		nuii		<u>coordinate data source code</u>
date_created	timestamp	8					
data madified	varunar	20	al		null.		
uale_moulleu userid_modified	varchar	0 20	শ		null		
usenu_moumeu	valullai	20	Ÿ		nuii		

The last table for examination and population is point_source_em. This table holds all the details on the actual emissions for the point source. Looking at this primary key we see that it has been built upon the previous tables by adding a few more fields to handle uniqueness criteria (Figure 12).

Figure 12. Keys for point_source_em.

Indexes:
Column(s)
country_code + state_county_fips + pt_facility_id + pt_eu_id + pt_process_id + pollutant_code + start_date + ef_reliability_indicator

Looking at the table definition we see that start_date is a table key much like pt_process_id that is only contained in point_source_em. The other two are in separate tables that need to be populated.

By following the linkages of tables from top to bottom, a complete data set for the SMOKE PTINV file can be entered. However, performing all that data entry by hand is very cumbersome if using the EIMA. The solution is to make a Comma Separated Value (CSV) file for each table and use a SQL utility to load the data into the database.

Bulk Data Loads

Bulk entry into the database can be done by using the SQL COPY command from the command line. To use this command the data must be in comma-delimited format with the column name at the top of each column. Through RTI's experience with importing data and from working with the client, we discovered that Excel would load, change, and export CSV files with the least effort. However, Excel occasionally leaves an odd character at the beginning of some strings. Therefore, the contents of each data file should be reviewed in a text editor (i.e., Notepad) before starting the import.

The database warns of any constraints not met while using the COPY command so understanding the requirements of each table before import is crucial. Many attempts may have to be made to import a single file as dependencies are checked and rechecked by the database's constraints.

For more information on the COPY command see the PostgreSQL user's guide here: <u>http://www.postgresql.org/docs/techdocs.15</u>. Syntax of COPY can be found here: <u>http://www.postgresql.org/docs/8.0/interactive/sql-copy.html</u>

CONCLUSIONS

Version 1 of the Emissions Inventory Maintenance Application (EIMA) has been successfully installed on the computers at BMEPB, where its user interface is Simplified Chinese language. It is also available in English, and can be translated to other languages without any reprogramming. The EIMA is licensed under the GNU Public License.

The data extraction utilities in the AQMDSS extract the emissions inventory data from the underlying database and create the input data files for SMOKE. Because all codes and related data are verified by EIMA during data entry, extremely few data problems can be expected when ingesting the data into SMOKE.

Finally, by using PostgreSQL as the database management system, the underlying emissions inventory database can be easily accessed by other programmers. Application programming interfaces are available for Java, C, C++, Perl, Python, and other languages. Also, the database can be directly accessed through SQL queries for ad hoc reporting. It also supports stored procedures, allowing additional, efficient data processing routines to be added to the AQMDSS in the future.

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