

# Process Optimization Guidance (POG and iPOG) for Mercury Emissions Control

Balaji Krishnakumar,<sup>†</sup> Stephen Niksa,<sup>\*,†</sup> Lesley Sloss,<sup>‡</sup> Wojciech Jozewicz,<sup>§</sup> and Gunnar Futsaeter<sup>||</sup>

<sup>†</sup>Niksa Energy Associates, LLC (NEA), Belmont, California 94002, United States

<sup>‡</sup>International Energy Agency (IEA) Clean Coal Centre (CCC), London SW15 6AA, United Kingdom

<sup>§</sup>ARCADIS, Research Triangle Park, North Carolina 27709, United States

<sup>||</sup>United Nations Environment Programme (UNEP), Geneva 10, Switzerland

**ABSTRACT:** This paper introduces two new tools to quickly identify and assess a broad range of Hg emissions controls for utility gas cleaning systems worldwide. The Process Optimization Guidance (POG) document summarizes the available options for mercury control at most coal-fired power plants, covering everything from efficiency improvements and fuel switching through co-benefit effects (maximizing Hg capture in existing pollution control systems) to Hg-specific sorbent and oxidation technologies. The POG includes a “decision tree” concept that helps the reader determine the potential compliance strategies for particular coal-fired gas cleaning systems. The Interactive Process Optimization Guidance (iPOG) is a user-friendly software package that formalizes the “decision tree” concept in the POG document. It accurately estimates Hg removals and emissions rates for broad ranges of coal quality, the most common configurations for furnace firing and flue gas cleaning, and Hg controls, both inherent and external. Two case studies presented in this paper show its utility in addressing “What if...?” scenarios, in which the impact of adding Hg controls to existing cleaning systems can be quickly and conveniently evaluated. The iPOG supports compliance strategies based on coal cleaning and blending, stronger inherent Hg removal in new air pollution control units for NO<sub>x</sub> and SO<sub>x</sub> control, and dedicated external Hg controls, such as activated carbon injection (ACI) and halogen addition. This flexibility is compounded by minimal input data requirements and extremely fast execution times. This makes the iPOG useful for those who are new to the technicalities within the issue of Hg control, such as policy makers or even operators in developed countries or countries with economies in transition. Relative novices can “play” with the iPOG, selecting generic coals and simple plant design options, and then discover just how much simple changes in coal characteristics or plant operation may affect emissions. Being based on statistical regressions of an American Hg field test database and streamlined input data requirements, iPOG cannot possibly resolve differences among different Hg control strategies within the measurement uncertainties or depict the distinctive features of particular gas cleaning systems. Such limitations are especially pronounced whenever SO<sub>3</sub> adsorption interferes with Hg removal via ACI and also when distinctive selective catalytic reduction (SCR) design specifications strongly affect Hg<sup>0</sup> oxidation along a SCR catalyst monolith. Whereas the Hg removals for such situations are accurately predicted by previously reported reaction mechanisms, they are beyond the current scope of iPOG. However, the iPOG is fully capable of estimating Hg emissions from a preferred control scenario ahead of expert analysis.

## ■ INTRODUCTION

In February 2009, the Governing Council of the United Nations Environment Programme (UNEP) agreed on the need to develop a global legally binding instrument on mercury. The negotiation of the text of the instrument, likely to be known as the Minamata Convention, is to be completed by 2013. To maximize the information available during negotiations, the Governing Council requested to “continue and enhance” the work of the UNEP Global Mercury Partnership. The partnership is regarded as one of the main mechanisms for the delivery of immediate actions on mercury during the negotiation of the global mercury convention.<sup>1</sup> The partnership currently has seven identified priorities for action (or partnership areas) that are reflective of the major source categories. One of these is the Coal Partnership. Because the behavior and control of mercury at coal-fired plants is complex, it is likely that developed countries and those with economies in transition will find it a significant challenge to act swiftly on mercury reduction strategies without expert guidance. In response to this, the Coal Partnership has produced the

Process Optimization Guidance document, known as the POG. The POG summarizes practices capable of providing reduction of mercury emissions from coal-fired power plants. The POG is a tool to help determine the approaches to control mercury emissions for individual coal-fired power plants, allowing for a preliminary selection of a mercury control strategy. The Interactive Process Optimization Guidance (iPOG) has been developed to allow users to investigate mercury behavior in coal combustion by changing parameters in a specially designed interactive computer model.

Both the POG and the iPOG are distributed as free tools for interested parties to help determine the most appropriate technologies for mercury control from coal combustion systems on a case by case basis.

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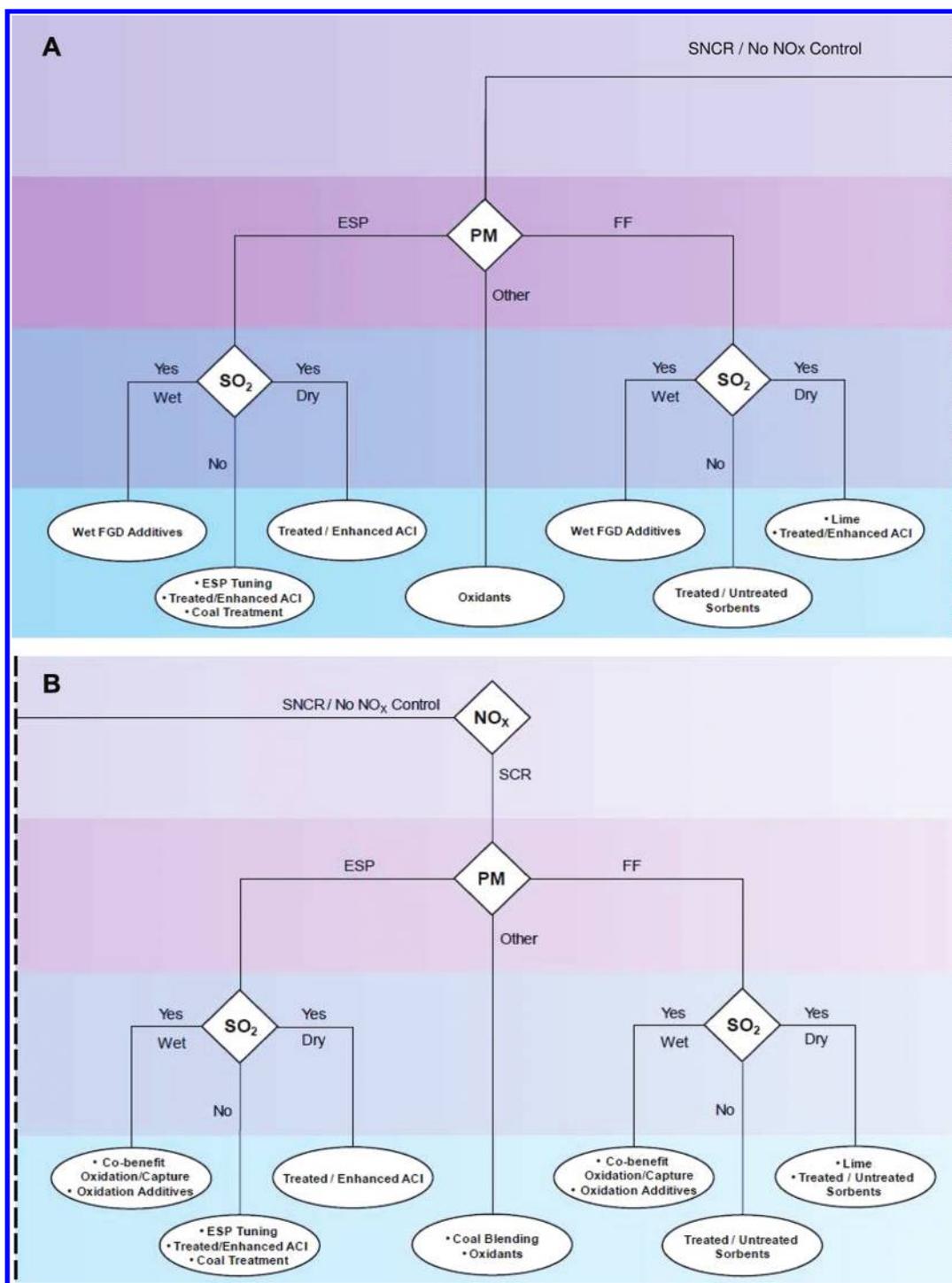


Figure 1. "Decision tree" diagram detail: (A) "SNCR/no NO<sub>x</sub> control" branch and (B) "SCR" branch.

## POG

The POG is intended to help users (plant operators, governments, policy makers, and any other interested parties) in evaluating potential opportunities to achieve multi-pollutant emission reductions, such as SO<sub>2</sub>, NO<sub>x</sub>, PM, and mercury emissions, including improved energy efficiency. The POG focuses on providing guidance on how to optimize plant performance and existing pollutant controls to achieve the co-benefits of reduced mercury emissions. However, the POG also includes information on mercury-specific control options, such as sorbent injection and oxidation strategies. The POG briefly

covers issues, such as mercury in ash and other residues, and how these should be handled. Because of the transient nature of such information and the rate at which the market is evolving, the POG does not include information of the costs of mercury control other than in a comparative manner (i.e., "high" versus "low" cost options).

To include specific experience in selected countries, workshops on the POG have been held in Russia, China, and South Africa and the document has been translated into Russian and Mandarin. The POG is available for free download from the UNEP Coal Partnership website.<sup>2</sup> As part of the POG,

the “decision tree” concept was developed summarizing the decision processes used to determine the most appropriate methods of mercury control on a case-by-case/plant-by-plant basis depending upon the NO<sub>x</sub>, PM, and SO<sub>2</sub> controls. This flow diagram is split into two in panels A and B of Figure 1 representing the branches with and without selective catalytic reduction (SCR).

The flow diagram is not diagnostic or prescriptive but rather aims to help the user focus on only those sections of the report that are relevant to their specific situation; i.e., those plants that already have SO<sub>2</sub> and NO<sub>x</sub> control systems are recommended to concentrate on oxidant techniques, whereas those plants with more basic pollution control systems in place have potentially more options to consider, including fuel switching, upgrading pollution control systems, and combined multi-pollutant control technologies, in addition to oxidant- and sorbent-based systems.

### ■ IPOG

The IPOG is a user-friendly software package that formalizes the “decision tree” concept in the POG document. Although the IPOG is not designed to provide a prescriptive determination of which control option is most appropriate at any particular plant, it does estimate the performance for various Hg control strategies and thereby focuses the user on only those options that are most relevant. The IPOG estimates Hg emissions rates from full-scale utility gas cleaning systems fired with any coal or coal blend, given a few coal properties, the gas cleaning configuration, selected firing and gas cleaning conditions, and an assortment of Hg control technologies. All of the most common gas cleaning configurations are implemented, and users can assess Hg emissions reductions by coal pretreatment and blending, the co-benefits to Hg capture from existing pollution control equipment for NO<sub>x</sub>, PM, and/or SO<sub>2</sub>, and Hg-specific control technologies, such as halogen addition with or without activated carbon injection (ACI) with untreated or brominated sorbents. Licensed commercial Hg control technologies, such as TOXECON-I and TOXECON-II and bromine addition, can also be examined. In addition, users can input coal properties from any geographical location in ranks from lignite to anthracite, alone or in blends of up to three components. The most common configurations and Hg control options are implemented as default selections in the IPOG, so that entry-level users can easily navigate toward the results. Experienced users can analyze advanced control configurations with their own detailed specifications. The estimated Hg emissions are primarily based on engineering correlations of the Hg field test database from American utilities, supplemented with predictions from Niksa Energy Associates LLC’s (NEA) detailed Hg transformation mechanisms, as explained later.

Because the simulations are cheap and fast, IPOG is a good tool to address “What if...?” questions regarding variations in fuel quality, cleaning configurations, operating conditions, and external Hg controls. The IPOG delivers quantitative answers to all of these types of questions in no more than a few seconds of execution time. The IPOG does not estimate the costs for the various compliance options. However, it nevertheless supports financial management strategies to minimize the costs of regulatory compliance by accurately estimating how much Hg can be removed for a broad range of inherent and external controls. When costs are associated with their Hg control scenarios, users will be in a position to identify the least

cost control options at the levels of individual plants as well as regional utility operations.

### ■ SCOPE OF THE CALCULATION SEQUENCE

Any calculation sequence to forecast Hg emissions using the IPOG proceeds through an intuitive sequence of up to seven interactive windows that resemble the screens in the Integrated Environmental Control Model.<sup>3</sup> The screens accept all required input specifications and present the estimated Hg speciation, the Hg collection efficiency for each air pollution control device (APCD), and the stack emissions. The gas cleaning configuration can be cold-side electrostatic precipitator (ESPC) only, fabric (or baghouse) filter (FF) only, hot-side electrostatic precipitator (ESPh) only, ESPh + FF, ESPC + FF, wet particulate matter (PM) only, SCR + ESPC, SCR + FF, SCR + wet PM, ESPC + wet flue gas desulfurization (WFGD), SCR + ESPC + WFGD, SCR + wet PM + WFGD, spray dryer absorber (SDA) + FF, SDA + ESPC, and SCR + SDA + FF. ESPC and/or FF in series can be configured for ACI between two PM control devices (TOXECON-I) or within an ESPC (TOXECON-II).

The allowable types of Hg control are collected in Table 1 and compared to the options included in the POG decision tree, as

**Table 1. Mercury Control Options in POG and IPOG**

| POG                                  | iPOG                                 |
|--------------------------------------|--------------------------------------|
| coal treatment                       | coal treatment                       |
| co-benefits for Hg oxidation/capture | co-benefits for Hg oxidation/capture |
| Hg <sup>0</sup> oxidation additives  | Hg <sup>0</sup> oxidation additives  |
| untreated ACI                        | untreated ACI                        |
| treated/enhanced ACI                 | treated/enhanced ACI                 |
| untreated non-carbon sorbents        |                                      |
| lime injection                       |                                      |
| ESP tuning                           |                                      |
| oxidants for wet PM                  |                                      |
| WFGD additives                       |                                      |

follows: (a) Coal treatment covers the elimination of pyrite and its associated Hg via both washing and float-and-sink separations. (b) Co-benefits for Hg oxidation and capture include in-flight oxidation and sorption of elemental Hg (Hg<sup>0</sup>) and oxidized Hg (Hg<sup>2+</sup>) on suspended unburned carbon (UBC) along ductwork, Hg<sup>0</sup> oxidation along SCR catalysts, collection of particulate Hg (HgP) on UBC in ESPs, oxidation of Hg<sup>0</sup> and collection of HgP on FFs, and retention of Hg<sup>2+</sup> in scrubbing solutions in WFGD (without Hg<sup>0</sup> re-emission). These Hg transformations may occur in any of the supported gas cleaning configurations. (c) Hg oxidation additives cover sprays of bromides and chlorides on the coal feed, as well as in-duct injections of Cl and Br vapors. (d) ACI can be implemented with both untreated and brominated carbons upstream of the air preheater (APH) and any particulate control device (PCD) and also within an electrostatic precipitator (ESP).

POG covers the following options that are not supported in IPOG: (1) non-carbon Hg sorbents, such as amended silicates, (2) ACI with lime co-injection in SDAs, (3) lime injection downstream of SDAs, (4) additives to promote Hg<sup>0</sup> oxidation in wet PMs and WFGDs, and (5) ESP tuning to enhance HgP capture. These controls cannot yet be supported in IPOG because the field test databases that cover broad ranges of fuel quality and cleaning configuration have not yet been reported. As more data on these approaches becomes available, they can be implemented.

Once a user specifies the cleaning configuration and Hg controls, if any, he or she then enters more detailed specifications on the cleaning conditions. Users new to Hg control technologies may use default specifications on coal rank and typical additive levels and ACI concentrations. Experienced users will enter the more detailed input specifications in Table 2. Single coals or coal blends with up to three blend components can be selected from any geographical location under any coal rank from lignite to anthracite. The listed coal

**Table 2. Input Data Requirements**

|                            |   |
|----------------------------|---|
| coal properties            | rank, moisture, ash, S, HHV, Cl, Hg, and blend percentages  |
| furnace conditions         | rating, load, gross efficiency, firing configuration, loss-on-ignition (LOI), economizer O <sub>2</sub> , and bottom ash (as a percentage of total ash) |
| gas cleaning configuration | flow diagram from the furnace exit to stack, including all APCDs and Hg controls  |
| SCR                        | economizer NO concentration and NO reduction efficiency   |
| ESP, FF, and wet PM        | PM collection efficiency  |
| WFGD and SDA               | SO <sub>2</sub> capture efficiency  |
| sorbent injection          | conventional or brominated sorbent, injection position, and concentration   |
| agent injection            | weight percentage halogen, injection position, and concentration  |

properties are used to estimate a flue gas composition. Under the best of circumstances, these properties should be reported for every day of Hg speciation measurements whenever iPOG estimates are compared to field test data. The iPOG covers the most common furnace firing configurations, including wall-, T-, and cyclone-fired furnaces. Stoker- or grate-fired furnaces and fluidized-bed combustors are not supported.

Furnace conditions are also required to estimate a flue gas composition and also to determine a flue gas flow rate. Given a furnace rating, a load profile during the tests, a higher heating value (HHV) of the fuel, and an O<sub>2</sub> concentration at the economizer, the gas flow rate and composition may be estimated on the basis of a specified gross thermal efficiency, which has a default value of 32%. The partitioning of coal ash into bottom ash and fly ash is also important because LOI is expressed as a percentage of the retained fly ash only. A NO concentration at the economizer must be provided whenever a SCR is present, along with the NO reduction efficiency. Only the overall PM collection efficiency must be specified, and these generally exceed 98%. Similarly, only the overall SO<sub>2</sub> capture efficiency of a WFGD must be specified. For both ACI and halogen additions, a chemical composition and the injection rate and position must be

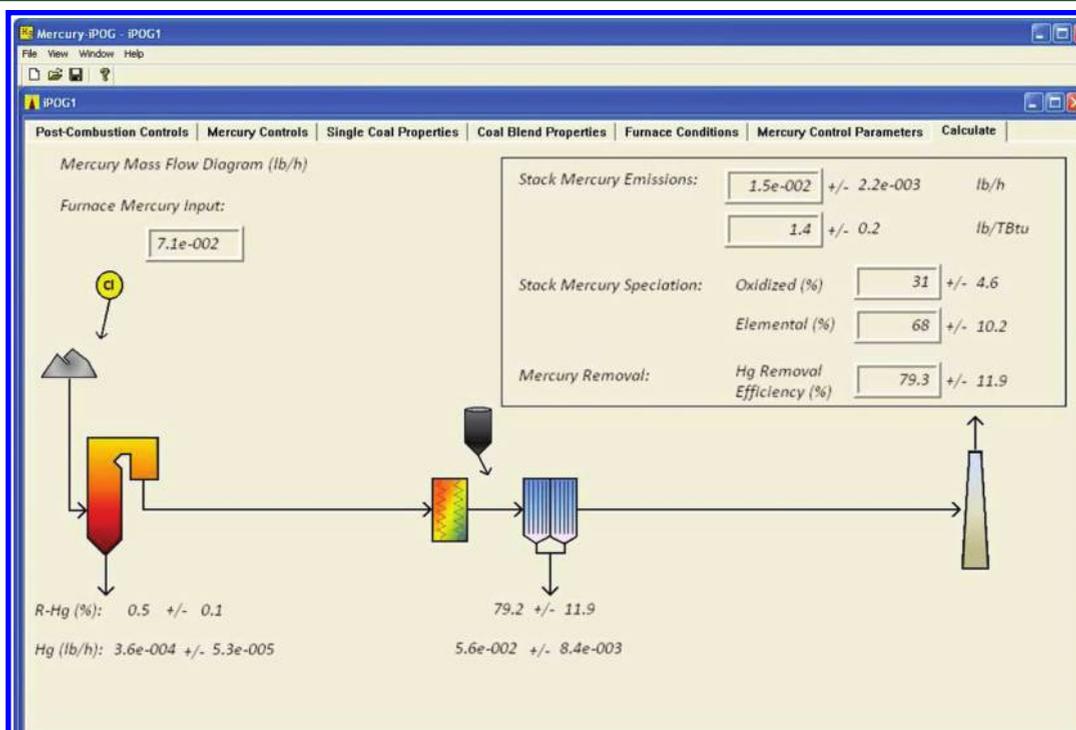
specified. Both conventional and brominated carbon sorbents are supported.

As seen in Figure 2, the calculation results comprise all Hg mass flows, Hg removals at all APCDs, and the Hg stack speciation and emissions for the selected gas cleaning and Hg control configuration. The mass flow rates of Hg in all input and exit streams appear along with the removals in individual APCDs along the gas cleaning system. For the test case shown in Figure 2 for chloride addition to the coal and ACI upstream of the ESP, users can parametrically vary the halogen and/or sorbent loadings and change the injection locations in a series of case studies to identify the best performance from this Hg control configuration.

## ESTIMATION ALGORITHMS

In the literature, Hg speciation and removal in utility gas cleaning systems have been estimated by statistical regressions of field test data, detailed chemical reaction mechanisms validated with field test data,<sup>4</sup> or some combination of the two.<sup>5</sup> Whereas the predictions from some chemical reaction mechanisms are generally accurate to within the measurement uncertainties,<sup>4</sup> reaction mechanisms must be supported by very thorough descriptions of the APCDs and cleaning conditions. Some of this information is proprietary, and some is not readily available, even to plant operators. Because the iPOG was designed to be used by non-technical policy analysts as well as emissions control specialists, the input requirements were kept to an absolute minimum, to deliver meaningful estimates for representative plant configurations rather than plant-specific predictions. This choice precludes any calculation sequence based on reaction mechanisms; therefore, the estimation algorithms in the iPOG are a series of APCD-specific regressions.

The database underlying the regressions was compiled primarily from the phase I and II U.S. Department of Energy (DOE)/National Energy Technology Laboratory (NETL) Mercury Control Technology Field Testing Program.<sup>6</sup> Phase



**Figure 2.** iPOG screenshot showing Hg emissions estimates for an ESPc only system with Cl addition and untreated ACI.

I characterized inherent Hg capture by testing at plants firing bituminous coals with SCRs and/or flue gas desulfurization (FGD) units in addition to ESPc. Phase II emphasized low-rank coals with ESPc only cleaning configurations supplemented by ACI.

Efforts in the past to describe Hg transformation and capture using statistical regressions based on the Information Collection Request (ICR) database of the U.S. Environmental Protection Agency (EPA) yielded poor quantitative performance.<sup>7–10</sup> These regressions are not statistically significant,<sup>8</sup> except for systems with SDAs, because of errors and omissions in the ICR database and inadequacies in the regression functions, among many other reasons.

We developed regressions to circumvent the two primary flaws in previous applications, which are (1) inherent discrepancies among measured values because of random variations in the gas cleaning conditions and (2) no database covers the entire range of coal quality and cleaning conditions for every gas cleaning configuration and Hg control option. To address these issues, we first qualified the reported Hg speciation components and Hg removals for consistency within  $\pm 15\%$  of the total Hg inventory across all sampling locations at each test site, as explained elsewhere.<sup>4</sup> Only qualified test data were used in the regressions. Then, the field test database was supplemented with predictions from the Mercurator software of NEA to bridge any major gaps in coal quality and cleaning conditions for each of the subject APCDs. Mercurator predictions were previously validated with the entire phase I and II NETL database within the measurement uncertainties, as well as with numerous other data sets from various utility companies. Formal evaluations with over 150 tests have already been reported.<sup>4,11,12</sup> On the basis of the satisfactory quantitative performance, we used Mercurator predictions to fill the gaps in the available measurements, particularly for wet PM and ACI into ESPh. The qualified database was then streamlined to exclude measurements and predictions that represent atypical APCD temperatures, flue gas residence times, etc., to minimize the impact of such unregulated variations.

The primary variables in the statistical regressions were selected to account for the most important parameters in the reaction mechanisms in Mercurator. They are the flue gas halogen concentration (Cl or Br), fly ash LOI, fly ash loading in the flue gas, specific surface area of the UBC, and ACI concentration. Product terms of the flue gas halogen level with the fly ash loading, UBC surface area, and ACI concentration were also included in applicable regressions. For systems with SCR, the NO concentration and the reduction efficiency were included. For systems with FGD, the regression variables were the fraction of Hg<sup>2+</sup> estimated for the FGD inlet and the SO<sub>2</sub> capture efficiency. The correlation coefficients for the Hg removals in the different APCDs and for the extents of Hg<sup>0</sup> oxidation across SCRs are presented in Table 3. For the three types of PCDs in the first three rows, the regressions account for variations in halogen levels because of both inherent coal Cl variations and the addition of external halogenation agents, along with fly ash loading, LOI, and UBC surface area. These correlation coefficients vary between 0.81 and 0.97. The comparable regressions for ACI into ESPc and FFs have coefficients from 0.83 to 0.93. The generally higher correlation coefficients for FFs versus ESPs suggests that random variations in the cleaning conditions are less consequential in FFs than in ESPs, probably because of the much greater contact areas between flue gas and the accumulated UBC in FF filter cakes.

**Table 3. Correlation Coefficients for iPOG Estimates with the NETL Database**

| APCD              | R <sup>2</sup> |
|-------------------|----------------|
| ESPc              | 0.83           |
| FF                | 0.97           |
| ESPh              | 0.81           |
| ACI + ESPc        | 0.83           |
| ACI + FF          | 0.93           |
| SCR <sup>a</sup>  | 0.76           |
| WFGD <sup>b</sup> | 0.83           |

<sup>a</sup>Hg<sup>0</sup> oxidation and not removal across the SCR. <sup>b</sup>WFGD Hg removal given the level of Hg<sup>2+</sup> at the WFGD inlet.

Correlation coefficients for wet PM and ESPh with ACI addition are omitted because no qualified measurements for these units were available in the database; therefore, these regressions are entirely based on Mercurator predictions.

The regression for SCRs is for Hg<sup>0</sup> oxidation and not Hg capture. It accounts for flue gas concentrations of NO and halogens, both Cl and Br, and the NO reduction efficiency across the SCR. The correlation coefficient for SCRs is 0.76, which is lower than the other control devices because Hg<sup>0</sup> oxidation across SCRs also depends upon the monolith type, the channel shape and size, and the catalyst porosity distribution and formulation. Whereas these aspects of the SCR design have been quantitatively related to the Hg<sup>0</sup> oxidation performance,<sup>13,14</sup> none of them factors into the iPOG estimates because they can be proprietary and are not readily available. Because Hg capture in WFGDs is primarily determined by the level of Hg<sup>2+</sup> entering the system and many factors upstream of the WFGD affect the inlet Hg<sup>2+</sup> level, we resolved WFGD retention, per se, by developing the WFGD regression from measured Hg<sup>2+</sup> levels at the WFGD inlet. The correlation coefficient of 0.83 therefore represents the agreement between measured and predicted Hg capture in the WFGD alone, without contributions from uncertainties in Hg<sup>2+</sup> predictions upstream of the WFGD. This regression also does not represent Hg<sup>0</sup> re-emission from WFGDs, as occurs infrequently and intermittently in some full-scale WFGDs.<sup>15</sup>

## ■ COMPARISON OF IPOG ESTIMATES WITH FIELD TEST DATA

The iPOG was developed to provide indicative results for populations of gas cleaning systems that describe “typical” cleaning conditions rather than plant-specific values. The supported cleaning configurations can be broadly classified as PCD only, PCD + FGD, SCR + PCD, and SCR + PCD + FGD. Each configuration can also be supplemented with external Hg controls from coal pretreatment, halogen addition, and/or ACI. The two most important variables affecting inherent Hg capture, coal Cl and fly ash LOI, can also be varied across the complete domain of commercial operation. iPOG results for all of these variations are compared to selected field test data in Table 4. The tolerances reported for the predictions provide the bounds of predicted values for a particular test case but do not represent the statistical accuracy of the predictions.

Wherever possible, tests with halogen addition and/or ACI were included for each cleaning configuration to extend the inherent variations in coal Cl and LOI. By necessity, the measurements behind these ranges came from different plants, which admit into these comparison variations in several other factors because of inherent differences among plant design and

Table 4. Comparisons of Hg Removals from iPOG to Selected Field Test Data

| coal              | test label | furnace | HCl (ppmv) | LOI (wt %) | halogen (ppmw)   | ACI (lb/MMacf) | measured (%) | iPOG estimate (%) |
|-------------------|------------|---------|------------|------------|------------------|----------------|--------------|-------------------|
| ESPc Only         |            |         |            |            |                  |                |              |                   |
| bit               | EES3U14    | T       | 90         | 5.9        |                  |                | 29.6         | 21.3 ± 3.2        |
| bit               | YAU2BL2    | T       | 19         | 9.0        |                  |                | 31.8         | 38.6 ± 5.8        |
| bit               | YAU22S2    | T       | 20         | 15.0       |                  | 4.2            | 71.6         | 65.0 ± 9.8        |
| sub-bit           | EES1U25    | cyclone | 4          | 15.0       |                  |                | 62.2         | 65.3 ± 9.8        |
| sub-bit           | PPU2BL2    | T       | 6          | 0.3        |                  |                | 7.6          | 10.5 ± 1.6        |
| sub-bit           | PPU2L8     | T       | 6          | 0.3        |                  | 4              | 56.8         | 47.8 ± 7.2        |
| lig               | MRYU2P3    | cyclone | 3          | 0.3        | 800 <sup>a</sup> |                | 10.5         | 10.8 ± 1.6        |
| lig               | MRYU2P4    | cyclone | 3          | 0.3        | 800 <sup>a</sup> | 0.5            | 16.2         | 16.4 ± 2.5        |
| sub-bit           | MEU2SE5    | T       | 5          | 1.5        | 190 <sup>b</sup> |                | 51.6         | 9.5 ± 1.4         |
| sub-bit           | MEU2SE6    | T       | 5          | 1.5        | 190 <sup>b</sup> | 2.9            | 69.3         | 41.8 ± 6.3        |
| sub-bit           | MEU2LH1    | T       | 5          | 1.9        |                  | 3 <sup>c</sup> | 94.8         | 95.0 ± 14.3       |
| TOXECON-I         |            |         |            |            |                  |                |              |                   |
| sub-bit           | PIU789P03  | wall    | 6          | 0.7        |                  | 1.0            | 70.4         | 66.7 ± 10.0       |
| sub-bit           | PIU789P23  | wall    | 6          | 0.7        |                  | 2.0            | 92           | 80.7 ± 12.1       |
| TOXECON-II        |            |         |            |            |                  |                |              |                   |
| sub-bit           | INU2PHG3   | T       | 6          | 0.45       |                  | 1.0            | 39           | 33.1 ± 5.0        |
| sub-bit           | INU2PHG5   | T       | 6          | 0.45       |                  | 6.0            | 65           | 57.9 ± 8.7        |
| ESPc + WFGD       |            |         |            |            |                  |                |              |                   |
| bit               | CON4U12    | wall    | 92         | 4.5        |                  |                | 85.2         | 79.1 ± 11.9       |
| blend             | MOUBL3     | wall    | 3          | 0.2        |                  |                | 24.6         | 45.1 ± 6.8        |
| blend             | MOUCL1     | wall    | 3          | 0.2        | 600 <sup>a</sup> |                | 51.7         | 68.9 ± 10.3       |
| lig               | MRYU2P4    | cyclone | 3          | 0.3        | 800 <sup>a</sup> | 0.5            | 45.4         | 38.6 ± 5.8        |
| lig               | MRYU2P8    | cyclone | 3          | 0.3        | 70 <sup>b</sup>  | 0.5            | 57.6         | 49.6 ± 7.4        |
| SCR + ESPc        |            |         |            |            |                  |                |              |                   |
| bit               | EES6U13    | T       | 85         | 3.5        |                  |                | 1.7          | 16.4 ± 2.5        |
| bit               | EES8U13    | T       | 40         | 2          |                  |                | 8.0          | 7.6 ± 1.1         |
| sub-bit           | MLRU4B4    | wall    | 6          | 0.25       |                  |                | 23.4         | 10.1 ± 1.5        |
| sub-bit           | MLRU4BR    | wall    | 6          | 0.25       | 50 <sup>b</sup>  |                | 22.5         | 9.3 ± 1.4         |
| SCR + ESPc + WFGD |            |         |            |            |                  |                |              |                   |
| bit               | EES2U21    | wall    | 40         | 0.75       |                  |                | 88.0         | 81.8 ± 12.3       |
| bit               | EES2U22    | wall    | 130        | 0.85       |                  |                | 88.9         | 88.4 ± 13.3       |

<sup>a</sup>CaCl<sub>2</sub>, <sup>b</sup>CaBr<sub>2</sub>, <sup>c</sup>Brominated ACI.

operation. Whereas these inadvertent variations can significantly affect Hg capture, they cannot affect the iPOG results. Consequently, the forthcoming comparisons to field test data are intended to demonstrate that the iPOG results can accurately depict the trends for variations in halogen levels, LOI, and ACI concentration, subject to the inevitable uncertainties that come into play whenever iPOG estimates are compared to the field test data from various plants.

The test cases for the ESPc only configuration cover lignite, sub-bituminous, and bituminous coals in T-fired and cyclone furnaces, with and without Cl/Br addition and with and without untreated and brominated ACI. The first three tests labeled EES3U14, YAU2BL2, and YAU22S2 depict large variations in coal Cl, LOI, and ACI concentrations to cover the entire commercial ranges of Cl and carbon surface areas. The measured Hg removals for the three cases of 30, 33, and 72% compare well to the iPOG estimates of 21, 39, and 65%, respectively. The next three tests represent sub-bituminous coals with very low Cl but a large range of carbon surface area because of large LOI variations of 15 and 0.3 wt % and a substantial ACI concentration. Even with very little Cl, ACI increased the Hg capture from approximately 8 (PPU2BL2) to 57% (PPU2L8), which is clearly evident in the iPOG estimates. The inherent capture with 15% inherent LOI (EES1U25) is even greater and also apparent in the iPOG estimate, even though cyclone furnaces give lower fly ash loadings and lower

LOI surface areas than T-fired furnaces. The next two cases, MRYU2P3 and MRYU2P4, represent very high Cl and carbon surface areas from a lignite coal fired in a cyclone furnace with CaCl<sub>2</sub> added on coal and, in one case, ACI at a low concentration of untreated carbon. As expected, the Hg removals as HgP are low both with and without ACI, and the iPOG estimates accurately depict the enhanced capture with ACI.

The final three measurements under the ESP only configuration are for the same T-fired furnace firing a sub-bituminous coal with the addition of Br as CaBr<sub>2</sub> and with untreated and brominated ACI. Whereas the measurements show significant levels of Hg capture because of CaBr<sub>2</sub> addition and CaBr<sub>2</sub> addition with untreated ACI at 2.9 lb/MMacf, the iPOG estimates are 30–40% lower. The estimated 9.5% Hg capture in MEU2SE5 is similar to the low Hg capture estimated for MRYU2P3 with the addition of 800 as-received (ar) ppmw CaCl<sub>2</sub>. Because Br addition does not increase HgP in field tests,<sup>16</sup> the high capture in MEU2SE5 without ACI points to either a measurement error or some atypical condition at this location. With Br addition and untreated ACI (MEU2SE6), the estimate is closer to the measured Hg removal, and the remaining discrepancy should probably be attributed to the very large discrepancy in the baseline case with only Br addition. In contrast, the near-complete Hg capture in the saturation limit for brominated ACI is accurately estimated for

case MEU2LH1. Because iPOG does not have any user-specified calibration factors, discrepancies in a baseline case will tend to propagate through case studies with added Hg controls, as illustrated in this case study.

Two more PM only configurations in Table 4 represent the licensed Hg control technologies of TOXECON-I and TOXECON-II, whereby ACI is positioned between an ESPc and a FF and within the fields of an ESPc, respectively. In the TOXECON-I tests, the measured Hg removals increased from 70 to 92% as the ACI concentration was increased from 1 to 2 lb/MMacf. The enhancement is also apparent in the iPOG estimates, albeit in terms of Hg removals that are too low by up to 11% (but within the uncertainties on the estimates in both cases). Most of the Hg capture in these cases was due to HgP capture in the FF filter cake, which is typically estimated more accurately than for other PM controls (cf. the very high correlation coefficient in Table 2). In the TOXECON-II tests, the measured Hg removals increased from 39 to 65% as the ACI concentration was increased from 1 to 6 lb/MMacf. This enhancement is also apparent in the iPOG estimates, which grew from 33 to 58% for the greater ACI concentration. Note that the iPOG estimates accurately depict the better performance of TOXECON-I compared to TOXECON-II, insofar as even a much greater ACI concentration in TOXECON-II could not achieve the performance of TOXECON-I with the same Cl levels, because FFs are the most effective collectors of HgP, by far.

The cases for an ESPc + WFGD cleaning configuration cover lignite and bituminous coals and bituminous/sub-bituminous blends for wall-fired and cyclone boilers with external Cl/Br addition and ACI. This configuration removes HgP in the ESPc and Hg<sup>2+</sup> in the WFGD. The iPOG estimates accurately depict how judicious applications of Cl and Br addition and ACI can enhance Hg removals with lignite (MRYU2P4 and MRYU2P8) into the realm of removals normally seen with bituminous coals (CON4U12). The estimates also accurately depict the enhanced removal with the blend because of Cl addition (MOUCL1), although the large discrepancy for the baseline removal (MOUBL3) has again propagated into the case with an external Hg control. The accurate estimates for the total Hg removals were not due to fortuitous compensation of erroneous removals for the ESPc and WFGD. Test MRYU2P4 appears in both the ESPc only configuration and the ESPc + WFGD configuration with the distinction that the measured Hg removal in the former case refers to the ESPc removal only, while the latter case denotes the combined Hg removal in the ESPc + WFGD system with in-furnace addition of 800 ar ppmw CaCl<sub>2</sub> and 0.5 lb/MMacf ACI upstream of the ESPc. The estimated ESPc Hg removal was accurate at 16 versus 16.2% measured, and the estimated overall Hg removal was accurate at 39 versus 45.4% measured. The benefits of adding a WFGD to an ESPc only cleaning system are clearly apparent in the iPOG estimates.

The next four comparisons are for the SCR + ESPc configuration, including one case with Br addition. All of the measured Hg removals and the iPOG estimates are less than 25%, because these cleaning systems have no WFGD to retain the Hg<sup>0</sup> that is oxidized to Hg<sup>2+</sup> in the SCR. The estimated removal is accurate for the bituminous case with the lowest Cl (EES8U13) but not for the case with much greater Cl and carbon surface areas (EES6U13). It may seem incorrect that the measured removal for the greater Cl and LOI is much lower than that for the lower acid concentrations. However, these

data were obtained at different furnaces and provide yet another illustration of the significance of plant-specific factors. Without a baseline calibration protocol, iPOG can only depict the established tendency for greater removals for progressively greater Cl and LOI levels. For the pair of sub-bituminous cases, iPOG correctly predicts no enhancement for Br addition, because Br addition does not enhance the production of HgP, the form of Hg removed in an ESPc. However, both estimates are low by almost 15%.

The NETL field test database on the SCR + ESPc + WFGD configuration covers only furnaces fired with bituminous coals because low-rank coals tend to have low coal S; therefore, plants firing low-rank coals typically do not require both SCR and FGD for NO<sub>x</sub> and SO<sub>2</sub> emissions compliance in the U.S.A. Despite the large variations in the Cl levels of the two test cases from the same plant in Table 4, the measured Hg removals were the same and the estimates increased by less than 10% for the greater Cl level and slightly greater LOI (EES2U22). This behavior is a consequence of a saturation in the impact of Cl variations on Hg removals that changes from a direct proportionality at low Cl levels to an insensitivity to Cl variations at high levels. That transition usually occurs around 25 ppm Cl in flue gas; therefore, both cases in Table 4 were within the saturation region.

To summarize, we note that the iPOG estimates correctly rank order the Hg removals for the different gas cleaning configurations. For typical cleaning conditions, the iPOG predicts the lowest levels of inherent Hg capture for the ESPc only and the SCR + ESPc configurations, albeit with very substantial enhancements for halogen addition and ACI provided that the Cl levels and carbon surface areas are reasonably balanced. Successively higher removals are predicted for the ESPc + WFGD and SCR + ESPc + WFGD configurations. The iPOG estimates also show that the only PM only cleaning configuration that can match the performance of an SCR + ESPc + WFGD is TOXECON-I.

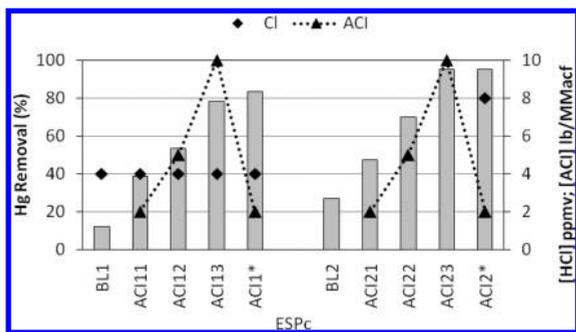
## PARAMETRIC CASE STUDIES

While the evaluations in Table 4 demonstrate the performance of iPOG across broad domains of coal quality, cleaning configurations, and Hg controls, the case studies in this section exploit that performance to examine representative “What if...?” questions.

**Case 1.** Rank order the Hg removals for coal blending, halogen addition, and/or ACI in an ESPc only configuration fired by sub-bituminous coal.

The baseline condition (BL1) is an ESPc only cleaning system fed by a 750 MW wall-fired furnace fired with sub-bituminous coal. The coal Cl is 0.01 ar wt %, which gives 4 ppmv HCl in the flue gas. The fly ash LOI is 0.75 wt %. According to iPOG, the ESPc removes 12% of the Hg (cf. case PPU2BL2 in Table 4). We next evaluate conventional ACI upstream of the ESPc, which gives removals of 38% for 2 lb/MMacf in case ACI11, 53% for 5 lb/MMacf in ACI12, and 78% for 10 lb/MMacf in ACI13. Higher ACI concentrations do not continue to increase the removals because the performance has become limited by the availability of Cl. To circumvent this constraint, we evaluate brominated ACI at 2 lb/MMacf in case ACI1\*, which removes 83% of the Hg. The removals from these five cases are collected in Figure 3, where the superior performance of brominated ACI is clearly apparent.

The next series is identical, except that the sub-bituminous coal was replaced by a 30:70 sub-bituminous/bituminous blend,



**Figure 3.** Parametric cases on Hg control options for a (left) sub-bituminous coal and a (right) sub-bituminous/bituminous coal blend in an ESPc only configuration. (\* denotes brominated ACI).

which gave 32 ppmv HCl and increased the LOI to 3.5 wt %. As seen in Figure 3 (five cases on the right), the baseline removal increased to 27% and the removals for the various ACI conditions also improved, on average, by approximately 15%.

**Case 2.** A plant firing bituminous coal into a SCR + ESPc + WFGD is modified to run on sub-bituminous coals or 50:50 bituminous/sub-bituminous blends. Identify halogen additions that give the same Hg removals as the baseline bituminous condition.

First, we determine the inherent Hg removal for a bituminous coal fired in a 750 MW wall-fired furnace with a SCR + ESPc + WFGD combination. The coal Cl is 0.054 ar wt %, which corresponds to a flue gas HCl of approximately 27 ppmv. The fly ash LOI is 3.5 wt %. The estimated Hg removal for this case was 84%. Analogous calculations for the sub-bituminous coal reduced the removal to 63% based on a coal Cl of 0.01 ar wt % and a fly ash LOI of 0.75 wt %. The baseline removal for the 50:50 blend was 76% based on a coal Cl of 0.035 ar wt % and a LOI of 2.5 wt %. We next estimated the removals for a series of progressively greater  $\text{CaCl}_2$  additions, first, on the sub-bituminous coal and, then, on the 50:50 blend. The entire series was then repeated with  $\text{CaBr}_2$  additions to the sub-bituminous coal and the 50:50 blend. These results are collected in Table 5.

**Table 5. Impact of Halogen Addition as  $\text{CaCl}_2$  or  $\text{CaBr}_2$  on a Sub-bituminous and a 50:50 Sub-bituminous/Bituminous Blend Fired into a SCR + ESP + WFGD**

| case          | $\text{CaCl}_2/\text{CaBr}_2$ (ppmw on coal) | coal Cl (ar ppmw) | Hg removal (%) |
|---------------|--|-------------------|----------------|
| bituminous    | 0  | 0.054             | 83.9           |
| PRB           | 0  | 0.010             | 63.3           |
|               | 50   |                   | 65.2           |
|               | 200  |                   | 70.8           |
|               | 400  |                   | 78.2           |
|               | 600  |                   | 85.6           |
|               | 50 Br  |                   | 74.8           |
|               | 100 Br                                       |                   | 86.5           |
| 50:50 PRB/Bit | 0  | 0.032             | 75.8           |
|               | 100  |                   | 79.0           |
|               | 300  |                   | 85.2           |
|               | 50 Br  |                   | 85.2           |
|               | 100 Br                                       |                   | 90.6           |

The bituminous coal gives a high inherent Hg removal of 84% because of its ample coal Cl, which promotes rapid  $\text{Hg}^0$  oxidation across the SCR and subsequent retention of nearly all of the  $\text{Hg}^{2+}$  in the WFGD. Conversely, the low coal Cl in the sub-bituminous coal diminishes the  $\text{Hg}^0$  oxidation performance of the SCR and thereby diminishes the inherent Hg removal to only 63%. Progressively greater  $\text{CaCl}_2$  additions restore the SCR performance, so that adding 600 ppmw  $\text{CaCl}_2$  to the sub-bituminous coal gives the same Hg removal as the bituminous baseline. The target is much easier to meet with the 50:50 blend, because both the coal Cl and LOI are greater (although UBC is much less effective in oxidizing  $\text{Hg}^0$  than the SCR under these cleaning conditions; therefore, LOI is a marginal consideration). Consequently, adding 300 ppmw  $\text{CaCl}_2$  to the blend provides sufficient Cl to obtain the Hg removal for the bituminous baseline. The impact of  $\text{CaBr}_2$  addition is analogous, albeit with much greater sensitivity. The removal for the bituminous baseline was achieved with only 100 ppmw  $\text{CaBr}_2$  on the sub-bituminous coal and 50 ppmw on the 50:50 blend.

### ■ LIMITATIONS ON THE HG EMISSIONS ESTIMATES

As stated before, the use of comprehensive reaction mechanisms to forecast Hg capture and emissions within useful quantitative tolerances require an inordinate amount of information on the fuels, furnace, and gas cleaning system. Because the POG and, now, iPOG were developed for a much broader user base, including people with no immediate experience in controlling Hg emissions, we definitely did not incorporate state-of-the-art calculation sequences to achieve the tightest quantitative accuracy on the calculation results. Trade-offs were deliberately made to eliminate all but the most basic input requirements at the expense of quantitative accuracy for any particular utility gas cleaning system. Obviously, these trade-offs limit how the estimates from the iPOG should be used.

The most general limitation is that the iPOG estimates are, for the most part, based on regressions of field test data. Users must therefore realize that these estimates are certainly no more accurate than the qualified measurement uncertainties, which we estimate at 10–15% of the total Hg inventory based on qualification of the NETL test data. Differences among cases that are smaller than these tolerances are certainly not statistically significant and should be ignored for the most part.

Another important limitation on the estimates is due to the omission of all but the gross cleaning conditions from the input data requirements, which ensures that iPOG cannot possibly depict the distinctive features of particular gas cleaning systems. Three instances of these system-specific omissions should be kept in mind. First, users do not specify the temperatures of their PM control devices. The production rate of HgP is fairly sensitive to the operating temperature of an ESPc or FF, yet all of the estimates from iPOG are for a nominal operating temperature of these devices in the U.S.A. In ACI applications, the estimates do not account for the variable performance of carbon sorbents from different vendors, because of differences in preparation techniques, loadings, and surface areas. Most importantly, the estimates for the capture of HgP on the UBC in LOI and also on carbon sorbents do not account for interference by adsorbed  $\text{SO}_3$ . This interference can cut Hg removals on untreated and brominated carbon sorbents in half under the worst circumstances (as shown below). Unfortunately, there are no useful empirical restrictions on the

interference by  $\text{SO}_3$ , because  $\text{SO}_3$  interference typically arises if the flue gas cools below its dew point in the APH and most power plant operators in the U.S.A. try to regulate their PM control temperatures to remain above these dew points. Whenever this threshold is breached, estimates from iPOG will substantially overpredict the Hg removals.

The second limitation from system-specific omissions pertains to the oxidation of  $\text{Hg}^0$  along SCR monoliths. The iPOG accounts for variations in the HCl and HBr concentrations in the flue gas, but it does not account for variations among the SCR design specifications and in the reactivities of the catalysts from different manufacturers and different lifetimes in service. Collectively, the variations in the SCR design specifications are at least as important as the variations in the halogen concentrations in the flue gas.<sup>13</sup> However, these design specifications had to be omitted from the iPOG because they pertain to deeply technical and often proprietary information that many utility companies do not even have. Again, the estimates from iPOG for cleaning systems with SCRs are for some nominal average set of SCR design specifications and are therefore subject to considerable uncertainties whenever they are applied to a SCR that operates away from these nominal specifications.

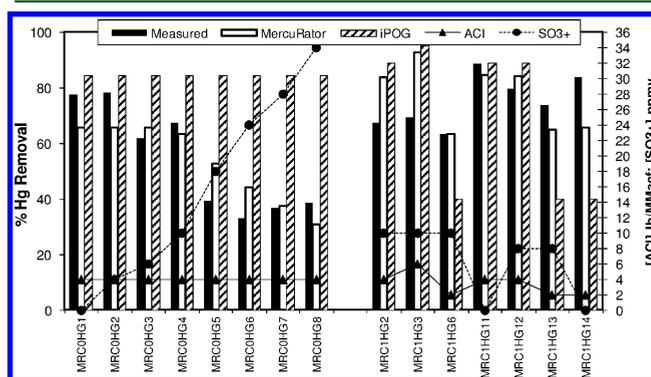
The third limitation from system-specific omissions pertains to the retention of  $\text{Hg}^{2+}$  in WFGDs. In most WFGD systems, essentially all of the  $\text{Hg}^{2+}$  in the inlet flue gas is retained in the scrubber wastewater or, occasionally, in the gypsum product. Rarely, however, significant fractions of the dissolved oxidized Hg are re-emitted as  $\text{Hg}^0$ . The factors responsible for re-emission have been identified, at least partially,<sup>15</sup> but again, they are too involved to incorporate into a tool like the iPOG. Consequently, iPOG users should realize that the relatively high Hg removals estimated for cleaning systems with WFGDs can represent significant overpredictions for the unusual situations where re-emission comes into play.

In a broader sense, many factors that affect Hg transformations vary among different utility gas cleaning systems. Examples include the length of ductwork among the APCDs, which affect reaction times, the temperatures and flue gas quench rates along the cleaning system, the deactivation of particular SCR catalysts by chemical poisons and mineral matter, the dispersion of injected sorbents and halogenation agents into the ductwork, and the cleaning cycles on PM collectors. Such factors can only be incorporated into simulation results by requiring calibration data on Hg emissions for baseline operating conditions, which are not required for the iPOG. The following examples illustrate the quantitative impact of these limitations on the iPOG estimates.

In the first case from the Mercury Research Center (MRC), Pensacola, FL, we demonstrate how MercuRator identifies the conditions under which  $\text{SO}_3$  inhibits Hg capture by carbon sorbents and predicts the extent of inhibition, which iPOG cannot do. As explained in more detail elsewhere,<sup>11</sup> the MRC is fed by a 5 MW flue gas slipstream from a 75 MW T-fired boiler burning either a South American coal or a blend of South American and Eastern bituminous coals. Two types of test configurations were used: (i) series MRC0,  $\text{SO}_3$  injected upstream of the APH with conventional ACI upstream of the ESP; and (ii) series MRC1, conventional ACI upstream of the APH and  $\text{SO}_3$  injected upstream of the ESP. In series MRC0, the ACI concentration was fixed at 4 lb/MMacf, while the added  $\text{SO}_3$  was varied from 0 to 34 ppmv. In series MRC1, the ACI concentration was varied from 2 to 6 lb/MMacf, while

the added  $\text{SO}_3$  was varied from 0 to 10 ppmv. The calculated acid gas dew points varied from 134 °C for the baseline 9.5 ppmv  $\text{SO}_3$  (with none added) to 150 °C for an additional 34 ppmv  $\text{SO}_3$ . The average ESP operating temperatures were 152 °C at the ESP inlet and 138 °C at the ESP outlet. In the MercuRator simulations,  $\text{SO}_3$  interference comes into play as soon as the flue gas temperatures fall below the acid gas dew point.

MercuRator predictions and iPOG estimates for Hg removals for the MRC tests are compared to the measured values in Figure 4. For series MRC0, MercuRator predictions exhibit the



**Figure 4.** Evaluation of Hg removals from MercuRator (open bars) and iPOG (cross hatched bars) with measured values (solid bars) for untreated ACI and  $\text{SO}_3$  additions at the MRC.

unperturbed Hg removals through 10 ppmv added  $\text{SO}_3$  and then diminish for progressively greater  $\text{SO}_3$  addition. They are accurate throughout the entire range of  $\text{SO}_3$  additions in these tests and clearly identify the conditions under which  $\text{SO}_3$  can diminish the Hg removals by ACI. In contrast, the iPOG estimates are the same for all  $\text{SO}_3$  levels and only express the variations in the ACI concentration. For series MRC1, the iPOG estimates are generally accurate for ACI at 4 lb/MMacf, but removals were significantly underestimated at 2 lb/MMacf and significantly overestimated at 6 lb/MMacf. MercuRator predictions for the tests with 2 lb/MMacf (MRC1HG3, MRC1HG13, and MRC1HG14) are within measurement uncertainties. The MercuRator predictions are within about 10% of the measured values in 12 of 15 tests, whereas the iPOG estimates are as accurate in only 4 of the 15 tests. Whenever  $\text{SO}_3$  inhibition comes into play, iPOG may significantly overestimate ACI performances, whereas MercuRator does not.

The second illustration pertains to  $\text{Hg}^0$  oxidation along SCRs. Detailed design specifications and operating conditions, in conjunction with flue gas halogen concentrations, are needed to accurately estimate extents of  $\text{Hg}^0$  oxidation across particular SCR units. The SCR submodel in MercuRator uses the detailed specifications in Table 6, whereas iPOG uses only the NO reduction efficiency and the inlet concentrations of NO and halogens. MercuRator quantifies the influences of the SCR temperature, gas hourly space velocity (GHSV), NO reduction efficiency ( $\eta_{\text{NO}}$ ), and the monolith type, physical specifications, and manufacturer. The underlying reaction and transport mechanisms cover the full domain of utility SCR conditions, with and without  $\text{NH}_3$  injection (during the non-ozone season) and reduced load operation.

For the conditions in Table 6, MercuRator predictions and iPOG estimates are compared to measured extents of  $\text{Hg}^0$  oxidation for several full-scale SCRs in Figure 5. This evaluation

Table 6. Input Specifications for Mercurator To Predict Hg<sup>0</sup> Oxidation along SCRs

|          | T (°C) | GHSV (h <sup>-1</sup> ) | average Cl (ppm) | NO (ppm) | $\eta_{NO}$ | catalyst          |            |                    |                     |
|----------|--------|-------------------------|------------------|----------|-------------|-------------------|------------|--------------------|---------------------|
|          |        |                         |                  |          |             | type <sup>a</sup> | pitch (mm) | shape <sup>b</sup> | vendor <sup>c</sup> |
| EES1U22  | 383    | 1800                    | 4                | 900      | 0.90        | H                 | 9          | S                  | COR                 |
| EES2U21  | 350    | 2125                    | 130              | 740      | 0.95        | P                 | 5.6        | C                  | ARG                 |
| EES2U2R1 | 350    | 2125                    | 40               | 415      | 0.95        | P                 | 5.6        | C                  | ARG                 |
| EES3U11  | 364    | 3930                    | 60               | 370      | 0.90        | H                 | 7.4        | S                  | KWH                 |
| EES4U13  | 363    | 2275                    | 50               | 730      | 0.91        | H                 | 8          | S                  | COR                 |
| EES4U1R3 | 363    | 2275                    | 15               | 600      | 0.91        | H                 | 8          | S                  | COR                 |
| EESU11   | 335    | 3700                    | 28               | 280      | 0.75        | P                 | 7.1        | T                  | HAT                 |
| EES6U11  | 375    | 3800                    | 79               | 330      | 0.85        | H                 | 9          | S                  | COR                 |
| EES8U13  | 336    | 3100                    | 49               | 530      | 0.94        | H                 | 9          | S                  | COR                 |
| CONSU12  | 356    | 2660                    | 105              | 375      | 0.94        | H                 | 7.1        | S                  | COR                 |
| CON10U21 | 356    | 2125                    | 40               | 355      | 0.88        | P                 | 5.6        | C                  | ARG                 |

<sup>a</sup>Honeycomb (H) or plate (P). <sup>b</sup>Square (S), rectangular (R), circular (C), or triangular (T) channels. <sup>c</sup>Cormetech (COR), Argillon (ARG), Halder-Topsøe (HAT), and KWH (KWH).

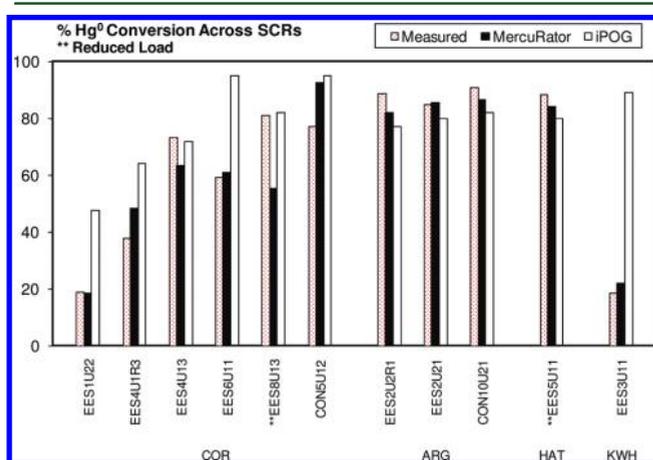


Figure 5. Evaluation of extents of Hg<sup>0</sup> oxidation across the SCRs in Table 6 from Mercurator (open bars) and iPOG (cross hatched bars) with measured values (solid bars).

covers temperatures from 335 to 395 °C, GHSV from 1800 to 3900 h<sup>-1</sup>, HCl concentrations from 1 to 130 ppm, inlet NO concentrations from 280 to 900 ppm,  $\eta_{NO}$  from 0.75 to 0.95, and four catalyst vendors. The Mercurator predictions are generally within 10% of the measured values for all cases, except EES8U13. The iPOG estimates depict the impact of variations in HCl and NO concentrations and  $\eta_{NO}$  but cannot describe variations in the SCR design specifications. Consequently, significant discrepancies arise for EES6U11, EES1U22, EES4U1R3, and especially, EES3U11.

## SUMMARY

We have demonstrated that the iPOG accurately estimates Hg removals and emissions rates for broad ranges of coal quality, gas cleaning configuration, and Hg controls. iPOG correctly estimates the rank order for the lowest levels of inherent Hg capture for the ESPc only and the SCR + ESPc configurations, albeit with very substantial enhancements for halogen addition and ACI, provided that the Cl levels and carbon surface areas are reasonably balanced. Successively higher removals are predicted for the ESPc + WFGD and SCR + ESPc + WFGD configurations. The iPOG estimates also show that the only PM only cleaning configuration that can match the performance of a SCR + ESPc + WFGD is TOXECON-I. Two case studies have shown its utility in addressing “What if...?”

scenarios, in which the impact of adding Hg controls, both inherent and external, to existing cleaning systems can be quickly and conveniently evaluated. iPOG supports the most common furnace firing configurations, gas cleaning configurations, and Hg controls; therefore, it is able to address a user's particular gas cleaning situation with an assortment of compliance strategies based on coal cleaning and blending, stronger inherent Hg removal in new APCDs for NO<sub>x</sub> and SO<sub>x</sub> control, and dedicated external Hg controls, such as ACI and halogen addition. This flexibility is compounded by minimal input data requirements and extremely fast execution times.

We have also tried to expose the inherent limitations of iPOG. On the basis of statistical regressions of an American Hg field test database, this program cannot possibly resolve differences among different Hg control strategies within the measurement uncertainties, which are almost never better than 10–15% of the total Hg inventory in any given test. It also cannot possibly depict the distinctive features of particular gas cleaning systems, because of the streamlined input data requirements and omission of a baseline calibration procedure. Moreover, a few potentially important but relatively infrequent influences on Hg emissions were omitted altogether, again, for the sake of streamlined input requirements. Such limitations are especially pronounced whenever SO<sub>3</sub> adsorption interferes with Hg removal via ACI and also when distinctive SCR design specifications strongly affect Hg<sup>0</sup> oxidation along a SCR catalyst monolith. Whereas the Hg removals for such situations are accurately predicted by detailed reaction mechanisms, such as Mercurator, they are beyond the current scope of iPOG.

## AUTHOR INFORMATION

### Corresponding Author

\*E-mail: neasteve@gmail.com.

### Notes

The authors declare no competing financial interest.

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## NOMENCLATURE

ACI = activated carbon injection  
APCD = air pollution control device  
DOE = U.S. Department of Energy  
ESP = electrostatic precipitator  
ESPc = cold-side electrostatic precipitator  
ESPh = hot-side electrostatic precipitator  
FF = fabric (or baghouse) filter  
FGD = flue gas desulfurization  
GHSV = gas hourly space velocity  
iPOG = Interactive Process Optimization Guidance software  
LOI = loss-on-ignition  
NEA = Niksa Energy Associates, LLC  
NETL = National Energy Technology Laboratory  
PCD = particulate control device  
PM = particulate matter  
POG = Process Optimization Guidance  
SCR = selective catalytic reduction for NO<sub>x</sub> control  
SDA = spray dryer absorber for flue gas desulfurization  
TOXECON = advanced sorbent injection configuration licensed by EPRI  
UBC = unburned carbon  
UNEP = United Nations Environment Programme  
WFGD = wet flue gas desulfurization

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