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Interactive Process Optimization Guidance

User Guide and Tutorial

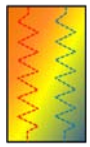
CONTENTS

ACRONYMS

ACI	Activated carbon injection.
APCD	Air pollution control device.
APH	Air preheater.
ESP	Electrostatic precipitator.
ESPc	Cold-side electrostatic precipitator.
ESPh	Hot-side electrostatic precipitator.
FF	Fabric (or baghouse) filter.
HHV	Higher heating value of the fuel.
iPOG	Interactive Process Optimization Guidance software.
NEA	Niksa Energy Associates LLC, the software developer.
LOI	Loss-on-ignition, as wt. loss after air oxidation of flyash.
PCD	Particle collection device.
PM	Particulate matter.
SCR	Selective catalytic reduction unit for NO_X control.
SDA	Spray dry absorber for flue gas desulfurization.
TOXECON	Advanced ACI configuration licensed by EPRI.
UNEP	United Nations Environment Program, the software sponsor.
WFGD	Wet flue gas desulfurization.

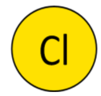
PROCESS FLOW DIAGRAM NOMENCLATURE

ACI



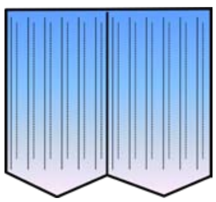
APH

Br Addition

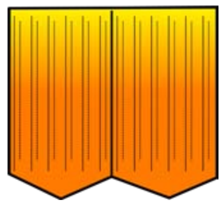


Cl Addition

Coal



ESPc



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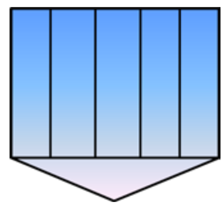

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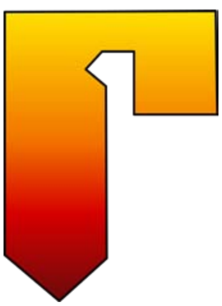
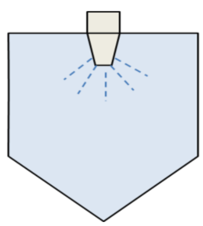


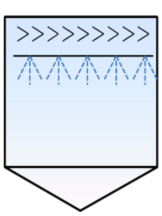
Furnace

SCR

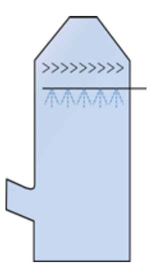


SDA

Stack



Wet PM



WFGD

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OVERVIEW

The Interactive Process Optimization Guidance (iPOG™) estimates the mercury (Hg) emissions rates and Hg speciation from full-scale gas cleaning systems on coal-fired utility boilers. This package was developed from January – July, 2011 by Niksa Energy Associates LLC (NEA) for the United Nations Environment Program, and is intended for unrestricted worldwide distribution. This *User's Guide and Tutorial* presents detailed instructions for estimating Hg emissions from utility power stations that burn any coal or coal blend in all the most popular gas cleaning configurations. This chapter surveys the main benefits, features, and functionality of the iPOG™.

What is the iPOG™ ?

The United Nations Environment Program (UNEP) previously developed and released its Process Optimization Guidance (POG) document to encourage the operators of coal-fired power plants in developing countries to assess their Hg emissions, and to contemplate an assortment of co-benefits from other air pollution control devices (APCDs) as well as from dedicated external Hg emission control strategies. The first version POG is in electronic text organized as a decision tree to guide users toward the Hg control options best suited to their particular utility operations (http://www.unep.org/hazardoussubstances/Mercury/MercuryPublications/GuidanceTrainingMaterialToolkits/tabid/3609/Default.aspx). Based on user feedback, UNEP wants to add value to POG by incorporating quantitative estimates of Hg emissions for existing gas cleaning configurations; for expanded systems with various contemplated APCDs; and with added external Hg controls. These estimates should be accurate enough to enable users to rank-order a broad assortment of options according to their extent of Hg reductions and ease of implementation.

The iPOG™is a user-friendly software package that predicts 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. It predicts the Hg emissions reductions for the most common inherent Hg controls, including systems with only particle collection devices (PCDs), and with ESP/FGD and SCR/ESP/FGD combinations. It also predicts Hg removals for injection of conventional carbon sorbents, brominated carbon sorbents, and halogenation agents, and estimates the Hg removals for different coal pretreatments. The estimated Hg emissions are based primarily on engineering correlations of the Hg field test database from American utilities, with support from NEA's detailed Hg transformation mechanisms.

Who Needs iPOG™ ?

- Utility compliance specialists and policy analysts will use iPOG™to run numerous "What If ?" scenarios across local and regional facilities. Ultimately, all these case studies could be synthesized into a strategy to achieve the greatest Hg emissions reductions for the lowest cost that are compatible with the company's specific constraints on coal quality and gas cleaning configuration, and the timetable and depth of impending Hg emissions regulations.

- Environmental managers will use it to estimate how modifications to a particular gas cleaning system will affect Hg emissions. The widespread installation of SCRs and FGDs currently underway in the USA and China is providing many opportunities to accurately estimate the reductions in Hg emissions rates due to retention of oxidized Hg in FGDs.

- Environmental and process engineers will use iPOG™to determine how variations in firing and gas cleaning conditions affect Hg emissions rates. Any adjustments to the firing conditions that significantly increase loss-on-ignition (LOI) levels, for example, may enhance Hg removals in the PCD.

- Fuel procurement specialists will use it to estimate Hg emissions rates for the range of coal quality in their current and foreseeable operations.

- Project engineers will use iPOG™ to ensure consistency with the backlog of data for similar gas cleaning configurations, and to understand where Hg is oxidized and removed along their gas cleaning system.

- OEMs for gas cleaning technology will use this package to estimate Hg emissions rates for their new installations. For example, FGD suppliers can easily estimate how much oxidized Hg is retained in the scrubber if they know the speciation at the FGD inlet. But that speciation is determined by the units upstream of the FGD, and iPOG™estimates the upstream Hg transformations.

We assumed that iPOG™ users are generally familiar with the terminology and unit operations in modern utility gas cleaning systems. But those new to Hg control technologies have two important resources to support their iPOG™ calculations: First, the POG document cited at the beginning of this chapter is an excellent introduction to the principles of Hg emissions control, and to the optimization strategies incorporated into the iPOG™. Second, all data entries in iPOG™can be made with default parameter specifications. Whereas entry-level iPOG™ users will heavily rely on the default specifications, expert users will take advantage of each input specification to tailor their simulation cases to match their existing and foreseen cleaning situations.

What Is iPOG™ Good For?

Since the simulations are cheap and fast, iPOG™ is a good tool to address "What if?" questions regarding variations in fuel quality, cleaning configurations, and external Hg controls. Will coal cleaning reduce Hg emissions by enough to meet the company's target for next year and beyond? What if the coal−Cl level surges by a factor of three or more in the primary supply mine, as we have seen in the field test literature? What if we add SCRs and FGDs to two base-load plants and only FGDs to three smaller plants? What will happen when those SCRs are taken out of service during specified seasons of a year? What if we applied activated carbon injection (ACI) at those three smaller plants instead of FGD? The iPOG™ delivers quantitative answers to all these types of questions in no more than a few minutes of execution time. Even if your curiosity is endless, this tool will keep pace.

The iPOG™ is also a means to extrapolate from a limited set of test data to the full ranges of coal quality and gas cleaning conditions across utility operations of any size and complexity. It is too expensive for a sizeable company to test all the important combinations of fuel quality and gas cleaning conditions in their current and foreseen operations. And data from one system is hard to directly apply to other systems of similar configuration because, inevitably, some of the important cleaning conditions were different in the test than they will be in the other systems. So the most efficient strategy is to first use a limited amount of test data to ensure that the iPOG™ results are accurate for the gas cleaning conditions of interest, then rely on iPOG™ to estimate Hg emissions rates for all the other fuels and gas cleaning configurations that will come into play among the similar cleaning configurations. Since computerized calculations are so much faster and cheaper than field testing, users can easily evaluate much broader ranges of Hg control conditions than are represented in a field test database.

The iPOG™ does not estimate the costs for the various compliance options that are analyzed. But 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. By associating costs with their Hg control scenarios, users will be in a position to identify least-cost control options at the levels of individual plants as well as regional utility operations.

System Requirements

The iPOG™ is a Microsoft Windows™-based, 32-bit application written in C/C++. The package is self-contained as a single executable file. No additional third-party software is required. It operates on systems that have the following minimum characteristics:

- A desktop or notebook personal computer using a Pentium processor or equivalent;
- 512 Mb RAM (1 Gb strongly recommended);
- A hard drive with 50 Mb of free disk space;
- Windows XP with Service Pack 2, Windows Vista or Windows 7;
- Screen resolution of at least 1024x768 pixels (1280x1024 or higher recommended).

Networked installations are not supported. If the GUI screens are too large, so that scroll bars are off-screen, change the screen resolution into the recommended range.

Software Installation

There is no formal installation procedure for the iPOG™, because it is distributed as a single executable file called "iPOGv10.exe." This file is completely self-contained, so that once it has been downloaded onto a user's hard drive or desktop, it is executed simply by clicking on its icon. Similarly, the iPOG can be uninstalled simply by deleting the executable file and all case and output files from the user's computer.

Input Data Requirements

To support entry-level users, default parameter specifications are available for every required input value in iPOG™, although experienced users will appreciate the opportunities to specify their actual cleaning conditions in the calculations. The input data requirements are collected in Table 1.1 according to the following groups:

(1) **Properties of the coal or coal blend** are required to estimate the flue gas composition. There are no means to accurately estimate Hg- or Cl-contents in coals. Coal properties should be reported for every day of Hg speciation measurements whenever predictions are compared to field test data.

Table 1.1.Input Data Requirements.

Coal Properties	Rank, Moisture, Ash, S, HHV, Cl, Hg, Blend Percentages
Furnace Conditions	Rating, Load, Gross Efficiency, Firing Configuration, LOI, Economizer O_2& Bottom Ash (% total ash)
Gas Cleaning Configuration	Flow diagram from furnace exit to stack, including all APCDs& Hg Controls
SCR	Economizer NO Concentration & NO Reduction Efficiency
ESP, FF, Wet PM	PM Collection Efficiency
WFGD, SDA	SO_2Capture Efficiency
Sorbent Injection	Conventional or Brominated Sorbent, Injection Position & Concentration
Agent Injection	Wt. Percentage Halogen, Injection Position & Concentration

(1) **Furnace conditions** are also required to estimate a flue gas composition, and also to determine a flue gas flowrate. Given a furnace rating, load profile during the tests, HHV, and O_2 concentration at the economizer, the gas flowrate and composition may be estimated, based on a specified gross efficiency, which has a default value of 32 %. The partitioning of coal ash into bottom ash and flyash is also important because LOI is expressed as a percentage of the retained flyash only.

(2) **Firing configuration** in terms of the sequence of APCDs is essential.

(3) **SCR conditions:**A measured NO concentration at the economizer must be provided whenever an SCR is present, along with the NO reduction efficiency.

(4) **PCD conditions:**Only the overall PM collection efficiency must be specified, and these generally exceed 98 %.

(5) **SO_2 Scrubber conditions:** Only the overall SO_2 capture efficiency must be specified.

(6) For both carbon **Sorbents and Halogenation Agents**, a chemical composition and the injection rate and position must be specified. Both conventional and brominated carbon sorbents are supported.

Steps to Estimating Hg Emissions

Any calculation sequence to forecast Hg emissions moves through the same sequence of steps. First, users provide information on the configurations of their furnace and cleaning system, along with a selection of operating conditions. Overall performance indices are needed on the APCDs that significantly affect the course of Hg transformations, such as PCDs, SCRs and WFGDs. They must also specify a selection of fuel properties that certainly includes coal rank, but may also cover a much broader range of characteristics. If users are interested only in the co-benefits of inherent Hg control that come automatically with the control technology for NO_X, SO_X, and PM emissions, they will then execute a calculation sequence to estimate Hg removals by various APCDs and the emissions released from the plant. Otherwise, users provide information about the external Hg controls that they want to consider, and then execute an expanded calculation sequence that properly accounts for the external controls.

In this latter sequence, there are potential options and constraints on the allowable fuel properties; the furnace types and firing configurations; the series of APCDs in the gas cleaning system and their operating domains; and the range of Hg control technologies. To the extent possible, we are trying to incorporate all the options included in the POG decision tree into iPOG™.

Once the input data have been assembled, users will open an iPOG™ session GUI consisting of seven tabscreens. They will move through the first 4 – 6 screens, depending on whether whole coals or coal blends are being fired and whether the case pertains to inherent or external Hg controls. When the GUI pages are complete, they then click on a final tab to execute iPOG™to estimate Hg emissions for the specified cleaning conditions. The execution time for each case is essentially instantaneous. The results of greatest interest are automatically entered into text file that can be archived under a name provided by the user. The following list summarizes the steps in estimating Hg emissions with this software:

1. Assemble the required input data.

2. Specify the gas cleaning configuration and all APCD specifications in the 'Post-Combustion Controls' window in the GUI.

3. Specify a coal pretreatment option and injection of either a carbon sorbent or a halogenation agent into the 'Mercury Controls' window in the GUI.

4. Enter fuel properties into the 'Single Coal Properties' window in the GUI.

5. If the fuel is a blend of components of different rank, formulate the blend properties in the 'Coal Blend Properties' window.

6. Enter the Hg control conditions in the ‘Mercury Control Parameters’ window if any external Hg controls were specified in step 3.

7. Execute iPOG™ by clicking on the ‘Calculate’ window, and immediately review the estimates for Hg speciation and removal by each APCD, as well as the stack Hg emissions rate and overall system Hg removal.

8. Archive the case under a user-specified name by renaming file ‘iPOG_Result.txt,’or by saving the entire session as a ‘.ipg’ extension file.

Organizationof This Manual

Each of the steps in the previous section is described in succeeding chapters. The required input data is restricted to the practical ranges of values given in Ch. 2, which also presents screenshots for complete calculation sequences. Chapter 3 presents a series of sample case studies to prompt iPOG™users to address the Hg emissions issues of greatest current interest to their companies.

Limitations on the Hg Emissions Estimates

Two decades of intensive research on Hg emissions from utility power plants, mostly in the Netherlands and USA, have identified a multitude of factors that affect the percentage of Hg in coal that is emitted through the smokestacks in large populations of utility power plants. The field test results were supplemented with basic knowledge from more controlled testing environments, and eventually synthesized into comprehensive reaction mechanisms that can forecast Hg emissions for particular power plants with specific coal samples within useful quantitative tolerances. Unfortunately, these mechanistic approaches require an inordinate amount of information on the fuels, furnace, and gas cleaning system, so they are not of much practical use to anyone without a depth of hard technical experience in utility emissions control. Since 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. Tradeoffs 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 tradeoffs 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, rather than on validated chemical reaction mechanisms. The bulk of the field test data came from the extensive program directed by the National Energy Technology Laboratory of the US Dept. of Energy. Generally speaking, this program designed its field tests to cover all the most important cleaning configurations and fuels, and the most popular Hg control technologies. Unlike typical corporate testing projects, each major NETL test series was documented with very detailed specifications on the fuel properties, test conditions, and the measurement uncertainties on the Hg speciation data. NEA also independently qualified each reported test for consistency with several established tendencies and with the apparent measurement uncertainties. Across the entire NETL database, about 15 % of all tests were rejected for model validation work, and these tests were also excluded from the statistical regressions developed for the iPOG™.

Notwithstanding such precautions, iPOG™ users must realize that the estimates from iPOG™ are certainly no more accurate than the qualified measurement uncertainties, which NEA estimates at 10 – 15 % of the total Hg inventory in each test. 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 need to omit all but the essential process characteristics from the input data requirements. Consequently, the estimates from iPOG™ cannot possibly depict the distinctive features of particular gas cleaning systems. Three particular instances of these system-specific omissions should be kept in mind. First, users do not specify the temperatures of their PM control devices. The recovery of particulate Hg (HgP) is known to be fairly sensitive to the operating temperature of an ESPc or FF, yet all the estimates from iPOG™ are for the nominal operating temperatures of these devices in the USA. In ACI applications, we also do not account for the variable performance of carbon sorbents from different vendors, due to differences in preparation techniques, loadings, and surface areas. Most important, the estimates for the capture of HgP on the unburned carbon in LOI and also on carbon sorbents does not account for interference by adsorbed SO_3. This interference can cut Hg removals on conventional and brominated carbon sorbents in half under the worst circumstances. Unfortunately, there are no useful empirical restrictions on the interference by SO_3, because SO_3 interference typically arises if the flue gas cools below its dew point in the air preheater (APH) and most power plant operators in the USA try to regulate their PM control temperatures to remain above these dew points. Whenever this threshold is breached, estimates from iPOG™ will express substantial over-predictions for the Hg removals.

The second limitation from system-specific omissions pertains to the oxidation of elemental Hg vapor (Hg^0) along SCR monoliths. The iPOG™ accounts for variations in the halogen concentration in the flue gas, in the concentrations of both HCl and HBr, but it does not account for variations among the SCR design specifications and in the reactivities of the catalysts from different manufacturers and of 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. But 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 an SCR that operates away from these nominal specifications.

The third limitation from system-specific omissions pertains to the retention of oxidized Hg vapor (Hg^{2+}) in WFGDs. In most WFGD systems, essentially all the 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 Hg^0. The factors responsible for re-emission have been identified, at least partially, 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 will represent significant over-predictions 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 halogenations 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 we are not requiring for the iPOG™.

Users who reach a point in their analyses with iPOG™ where these limitations are hindering their development work on Hg control strategies can consider more comprehensive simulation tools. NEA's MercuRator™ package is one such tool that requires system-specific input specifications and also uses field-test data to calibrate baseline predictions. A sample of the detailed input requirements for system-specific simulations in MercuRator™ appear in Table 1.2. Many of these input data such as SCR catalyst properties, sorbent characteristics and others are proprietary and may not be readily available to plant operators. iPOG™ users will appreciate the requirement of only a few input parameters, as outlined in Table 1.1, and yet obtain meaningful predictions of Hg speciation and capture, provided that they associate the results with groups of similar cleaning systems rather than a particular system.

Since MercuRator™ uses detailed chemical reaction mechanisms to simulate Hg transformations continuously from the furnace exit to the stack, through each APCD and between successive APCDs in a subject gas cleaning system, it circumvents some of the limitations mentioned in this section. Two cases studies illustrate the quantitative impact.

Table 1.2. Input Data Requirements for NEA's MercuRator™ software package.

	Essential	Helpful
Coal Properties	Moisture, Ash, S, HHV, Cl, Hg, blend percentages and properties	C, H, O, N
Furnace Conditions	Rating, Load, Economizer O_2& NO Bottom ash (% total ash)	Coal feedrate or gross thermal efficiency, economizer SO_2, HCl
Gas Cleaning Configuration	Flow diagram from furnace exit to stack, including all heat exchangers and APCDs	
Thermal History	FEGT, Economizer T, SCR T, Air Preheater Inlet T, ESP or FF T, FGD T	Nominal residence times for all heat exchangers and APCDs
SCR	GHSV at 32°F, inlet and outlet NO or molar NH_3/NO, T, pitch, channel shape, configuration, and vendor	Inlet and outlet T, monolith length, catalyst composition, pore size distribution
ESP	Flyash LOI, ESP temperature	Ash collection efficiency, residence time, SCA
FF	Flyash LOI, Air-to-Cloth, Cell number	Fabric material, cleaning interval and method
Wet FGD	Limestone slurry or Mg/Lime, inlet O_2, SO_2 capture efficiency, T	Molar Ca/S, solid product, inlet SO_2 and HCl
SDA	Slurry injection rate and composition, inlet O_2, SO_2 capture efficiency, T	Molar Ca/S, spray injector layout
Sorbent Injection	Type, total surface area, injection rate, location, temperature, and stream composition	Sorbent PSD
Agent Injection	Chemical composition, injection rate, location, temperature, and stream composition	

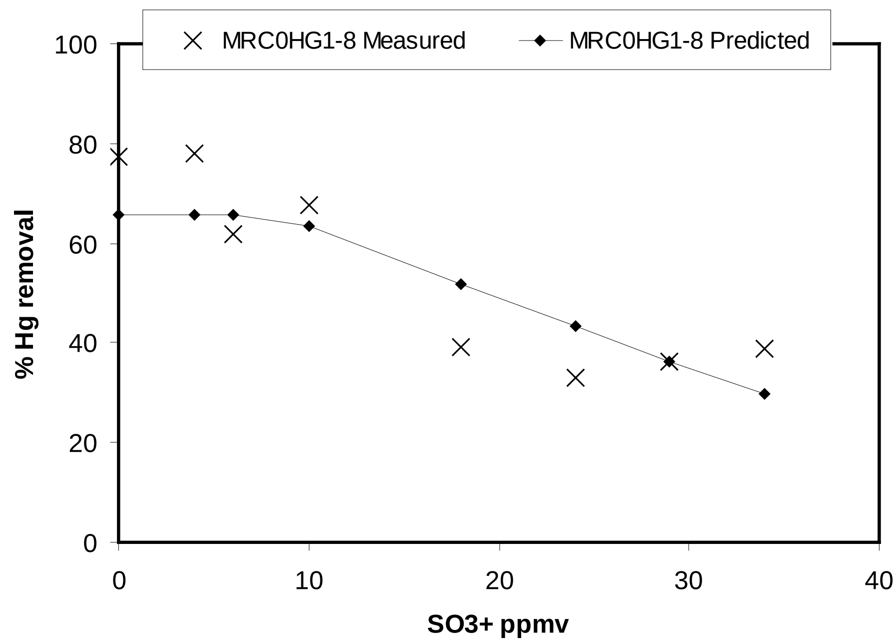


Figure 1-1.Comparison of NEA's MercuRator™ predictions with measured values at the MRC tests for SO_3 inhibition of Hg capture on ACI.

In the first case from the Mercury Research Center (MRC), Pensacola, FL, USA, the input data and the fundamental reaction mechanisms in MercuRator™ identify the conditions under which SO_3 inhibits Hg capture by carbon sorbents and predicts the extent of inhibition (which iPOG™ omits). 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. A series of eight tests evaluated the Hg removals for Darco Hg ACI both in the presence and absence of SO_3. The added SO_3 concentration in the flue gas, denoted by 'SO3+', was varied from 0 to 34 ppmv, while the ACI concentration was fixed at 4 lb/MMacf and the carbon was injected upstream of the ESP. The calculated acid gas dew points varied from 134°C for the baseline 9.5 ppmv SO_3(with none added) to 150ºC for an additional 34 ppmv SO_3. The average ESP operating temperatures were 152ºC at the ESP inlet and 138ºC at the ESP outlet. In the MercuRator™ simulations, SO_3 interference comes into play as soon as the flue gas temperatures fall below the acid gas dew point.

MercuRator™ predictions for Hg removals for the eight tests are compared with the measured values in Fig. 1-1. The predictions exhibit the unperturbed Hg removals through 10 ppmv added SO_3, then diminish for progressively greater SO_3 addition. They are accurate throughout the entire range of SO_3 additions in these tests and clearly

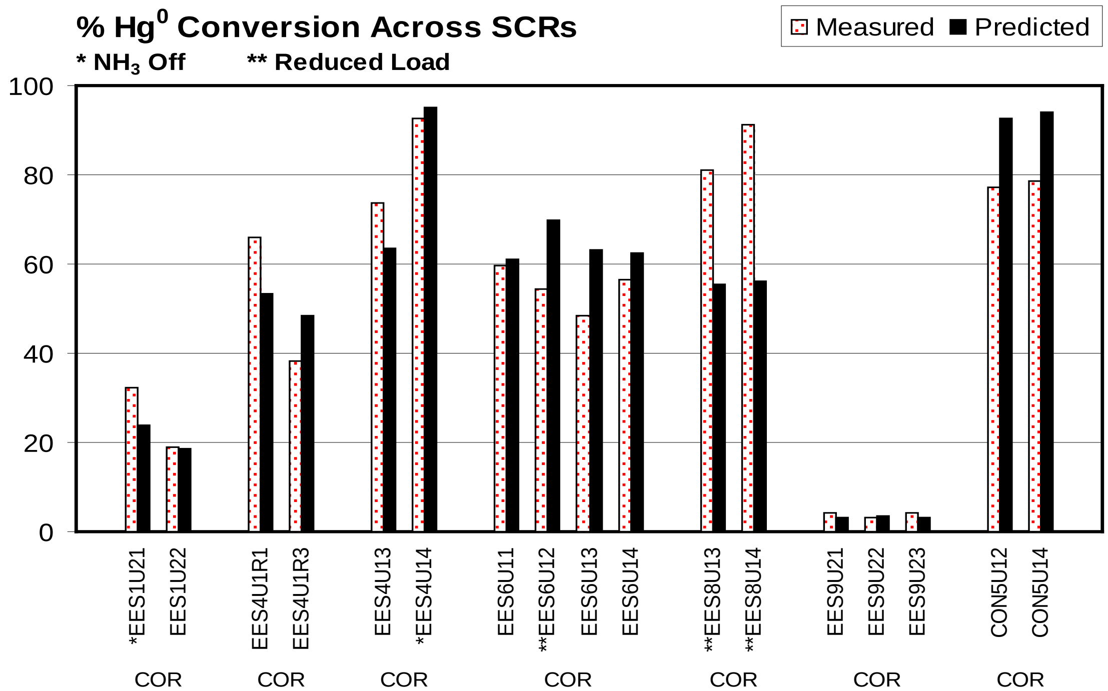
Table 1.3. Conditions for the SCR validations in NEA's MercuRator™.

	T °C	GHSV hr^{-1}	Avg. Cl,ppm	NO, ppm	η_{NO}	Catalyst			
						Type[a]	Pitch, mm	Shape[b]	Vendor[c]
S1	383	1800	4	900	0.90	H	9	S	COR
S2-1	350	2125	130	740	0.95	P	5.6	C	ARG
S2-2	"	"	40	415	"	"	"	"	"
S3	364	3930	60	370	0.90	H	7.4	S	KWH
S4-1	363	2275	50	730	0.91	H	8	S	COR
S4-2	"	"	15	600	"	"	"	"	"
S5	335	3700	28	280	0.75	P	7.1	T	HAT
S6	375	3800	79	330	0.85	H	9	S	COR
S8	336	3100	49	530	0.94	H	9	S	COR
S9	395	2800	<1	374	0.92	H	8.2	S	COR
CON5	356	2660	105	375	0.94	H	7.1	S	COR
CON10	356	2125	40	355	0.88	P	5.6	C	ARG

[a]Honeycomb (H) or plate (P).
[b]Square (S), rectangular (R), circular (C), or triangular (T) channels.
[c]Cormetech (COR), Argillon (ARG), Halder-Topsoe (HAT), KWH (KWH).

identify the conditions under which SO_3 can interfere with the ACI capture of Hg. But the iPOG™ does not account for any interference by SO_3, so the estimated Hg removals for ACI will represent upper limits. Additional MercuRator™ predictions for SO_3 inhibition of Hg capture on carbon sorbents have been validated against field-test data from several plants and for diverse conditions including bituminous, subbituminous coals and coal blends, and untreated and brominated ACI. These validations are published in the scientific literature and can be obtained via NEA's contact on this User Guide.

Similarly, detailed design specifications and operating conditions of SCR catalysts are required, in addition to flue gas Cl concentration, to accurately describe Hg^0 oxidation across individual SCR catalysts. As can be observed from Tables 1.1 and 1.2, the SCR specifications for MercuRator™ are significantly more complex and detailed than those for the iPOG™. Based on this detailed input and fundamental reaction mechanisms, NEA's MercuRator™ predicts the extent of Hg^0 oxidation across full-scale SCRs within useful quantitative tolerances. In addition to quantifying the effect of SCR temperature, gas hourly space velocity (GHSV), NO reduction efficiency (η_{NO}), catalyst type and



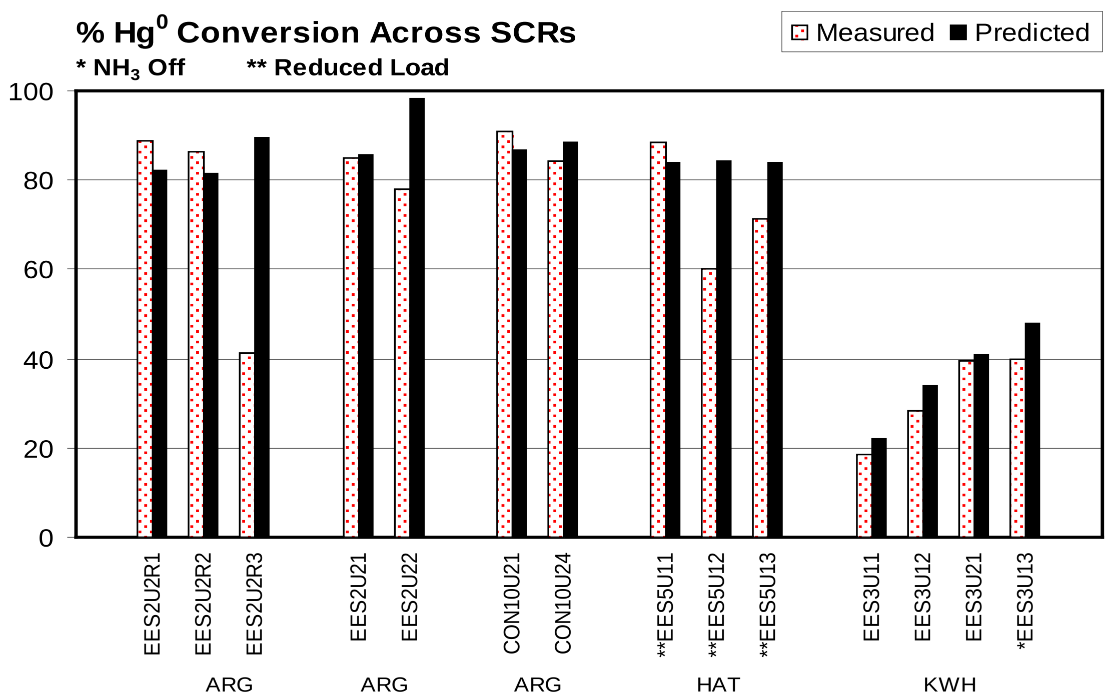


Figure 1-2. Validation of predicted extents of Hg^0 oxidation from MercuRator™ across full-scale SCRs with and without NH_3 injection for four catalyst vendors (COR, ARG, HAT and KWH).

Table 1.4.Measured and iPOG predicted™ SCR Hg^0 oxidation.

	T °C	GHSV hr^{-1}	HCl,ppm	NO, ppm	η_{NO}	Vendor[a]	Hg Oxd. (%)
EES4U13	363	2275	26	730	0.91	COR	72[b]
EES5U11	335	3700	28	280	0.75	HAT	88[b]
EES3U11	364	3930	45	370	0.90	KWH	18[b]
iPOG™-S4	-	-	26	730	0.91	-	73[c]
iPOG™-S5	-	-	28	280	0.75	-	80[c]
iPOG™-S3	-	-	45	370	0.90	-	89[c]

[a]Cormetech (COR), Halder-Topsoe (HAT).
[b]Measured; [c]Predicted.

physical dimensions, the predictions also account for the termination of NH_3 injection during non-ozone season and reduced load operating conditions. MercuRator™ predictions are compared with measured values of Hg oxidation for several full-scale SCR catalysts in Fig. 1-2. The detailed operating conditions for the SCR catalysts appear in Table 1.3. Note that the HCl concentrations in the table are averages of the measured value of several tests and the predictions account for the variations in HCl during individual tests within the same plant. For these tests, the operating temperatures varied from 335 to 395°C; space velocity from 1800 to3900 per hour; HCl concentration from 1 to 130 ppm; inlet NO concentration from 280 to 900 ppm; and η_{NO} from 0.75 to 0.95. For the qualified data, the correlation coefficient on the predictions is 0.91 and the standard deviation is 12.7 %.

The measured and predicted values show that the flue gas HCl concentration exerts a strong effect on the oxidation of Hg^0 across the SCR and, if all other operating conditions are constant, the SCR Hg^0 oxidation increases with increasing HCl. Yet, the SCR physical characteristics and operating conditions are at least as important as HCl in predicting catalyst-specific Hg^0 oxidation. For example, the tests EES4U13and EES5U11 have very similar HCl concentrations of approximately 27 ppmv, but the measured Hg^0 oxidation varied between 72 and 88 %. In contrast, the test EES3U11 has a higher HCl concentration of 45 ppm but shows a much lower Hg^0 oxidation of 18 %. The MercuRator™ predictions for all three cases are within the measurement uncertainty. The variation in the Hg^0 oxidation for these cases is attributed to differences in the catalyst manufacturers (cf. Table 1.3) and operating conditions, collected in Table 1.4. The iPOG™estimates of Hg^0 oxidation for S4 and S5 (comparable to tests EES4U13 and EES5U11) compare well with the measurements, at 73 vs. 72 % for S4 and at 80 vs. 88

% for S5. But the iPOG™estimate for S3 (comparable to test EES3U11) of 89 % SCR Hg^0 oxidation is, however, significantly different than the measured value of 18 %. The iPOG™ results convey the impacts of HCl and NO concentrations and η_{NO} for these cases with meaningful accuracy, but they cannot describe variations in the SCR design specifications. Whereas the iPOG™ provides meaningful predictions based on a limited set of input data and accounts for the effect of many of the major factors, users seeking plant-specific predictions would require more sophisticated models like MercuRator™ that account for all of the system-specific factors affecting Hg transformations.

Software specifications and extensive publications on the validation work behind MercuRator™ predictions can be obtained via NEA's contact information in this User Guide.

2

RUNNING iPOG™

Operating Modes in the iPOG™

There are two independent operating modes in the iPOG™, one for entry-level users and one for users with direct experience in gas cleaning systems, in general, and Hg emissions, in particular. Accordingly, each screen in the GUI contains only one register for entry-level users that retrieves blocks of input specifications under labels for various default options. This register is distinguished from all others by a generic, functional label, and by its position in either the top row or left side of a screen. Each screen also contains numerous additional registers for experienced users which are bounded by boxes whenever possible.

Scope of the Calculation Sequences

Any calculation sequence to forecast Hg emissions moves through the same sequence of steps. First, users provide information on the configurations of their furnace and cleaning system, along with a selection of operating conditions. More detailed specifications are needed on the APCDs that significantly affect the course of Hg transformations, such as SCRs, PM controls, and WFGDs. They must alsospecify a selection of fuel properties that certainly includes the coal rank and the Hg- and Cl-contents, but may also cover a broader range of characteristics. If users are interested only in the co-benefits of inherent Hg control that come automatically with the control technology for NO_X, SO_X, and PM emissions, they will then execute a calculation sequence to estimate Hg removals by various APCDs and the emissions released from the plant. Otherwise, users provide information about the external Hg controls that they want to consider, and then execute an expanded calculation sequence that properly accounts for the external controls.

In this sequence, there are potential options and constraints on the allowable fuel properties; the furnace types and firing configurations; the series of APCDs in the gas cleaning system and their operating domains; and the range of Hg control technologies. To the extent possible, we are trying to incorporate all the options included in the POG decision tree into iPOG™. The allowable options for fuels, furnace type, and firing configuration are as follows:

Table 2.1.MercuryControl Options in POG and iPOG™.

POG	iPOG™
Coal Treatment	Coal Treatment
Co-Benefits for Hg Oxidation/Capture	Co-Benefits for Hg Oxidation/Capture
Hg^0 Oxidation Additives	Hg^0 Oxidation Additives
Untreated ACI	Untreated ACI
Treated/Enhanced ACI	Treated/Enhanced ACI
Untreated Sorbents	
Lime Injection	
ESP Tuning	
Oxidants for Wet PM	
WFGD Additives	

(1) Fuels can be neat coals from any geographical region or blends of up to three such coals. Biomass, pet cokes, and all other opportunity fuels and their blends with or without coal are not supported.

(2) The major types of pulverized coal furnaces are supported, including front-wall, opposed-wall, T- or corner fired, cyclone, arch, and turbo. However, stoker or grate-fired furnaces, AFBCs, and CFBCs are not.

(3) Furnaces with overfire air, low-NO_X burners, selective non-catalytic reduction, and other forms of aerodynamic NO_X abatement are not supported. In-furnace sorbent injection for SO_X control is not supported.

(4) The gas cleaning configuration can be ESPc-only; FF-only, ESPh-only; ESPh+FF; ESPc+FF; Wet PM-only; SCR+ESPc; SCR+FF; SCR+Wet PM; ESPc+WFGD; SCR+ESPc+WFGD; SCR+Wet PM+WFGD; SDA+FF; SDA+ESPc; and SCR+SDA+FF.

The allowable types of Hg control are collected in Table 2.1 and compared with the options included in the POG decision tree. The following are the allowable options:

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 Hg^0 and Hg^{2+} on suspended unburned carbon (UBC) along ductwork; Hg^0 oxidation along SCR catalysts; collection of HgP on UBC in ESPs; oxidation of Hg^0 and collection of HgP on FFs; retention of Hg^{2+} in scrubbing solutions in WFGD (without Hg^0 re-emission). These Hg transformations may occur in any of the supported gas cleaning configurations(although POG did not cover ESPc-only systems).

c) Hg oxidation additives cover applications of bromides and chlorides on the coal feed, as well as in-duct injections of Cl- and Br-species.

d) ACI can be implemented with both untreated and brominated carbons upstream of the APH and any PCD, and also within an ESP.

In addition to the above four external Hg controls, 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^0 oxidation in Wet PMs and WFDGs; and (5) ESP tuning to enhance HgP capture. These controls cannot yet be supported in iPOG™ because the field-test databases that cover the necessary ranges of fuel quality and cleaning configuration have not yet been reported. As more data on these approaches becomes available, they can be added to the supported controls in iPOG™.

GUI Implementation

In the POG, the decision tree helps users to select and optimize their Hg control strategy by rank-ordering how APCDs for the control of NO_X, PM and SO_2 affect Hg emissions, and whether or not external Hg controls should be considered. In iPOG™, we use an intuitive step-by-step process to configure a user's actual and conceivable cleaning systems and Hg controls, and then provide quantitative estimates to further guide their selections. For each of the steps, the interface includes two modes of operation in the same screen. The first mode for entry-level users relies on default selections for the most common APCDs and Hg controls and operating conditions. This mode also allows users to familiarize themselves with the options available to more experienced users. The other mode is suited for more experienced users and features numerous customizable options. We first describe the general layout of the interface, then follow with more detailed descriptions of the configuration options on each screen.

Getting Started

Regardless of the operating mode, users will activate the iPOG™ by typing the program name into a command line, or by clicking on its icon from any resident location. Once activated, the program will bring up the main interface called the 'Parent Window,' which appears in Fig. 2-1. This window contains a few of the standard menu items in Windows applications, along with a toolbar along the top and statusbar along the bottom. A calculation sequence can be initiated from the menu or the toolbar. To initiate a new session from the menu, the user navigates through the 'File' menu and selects 'New' or

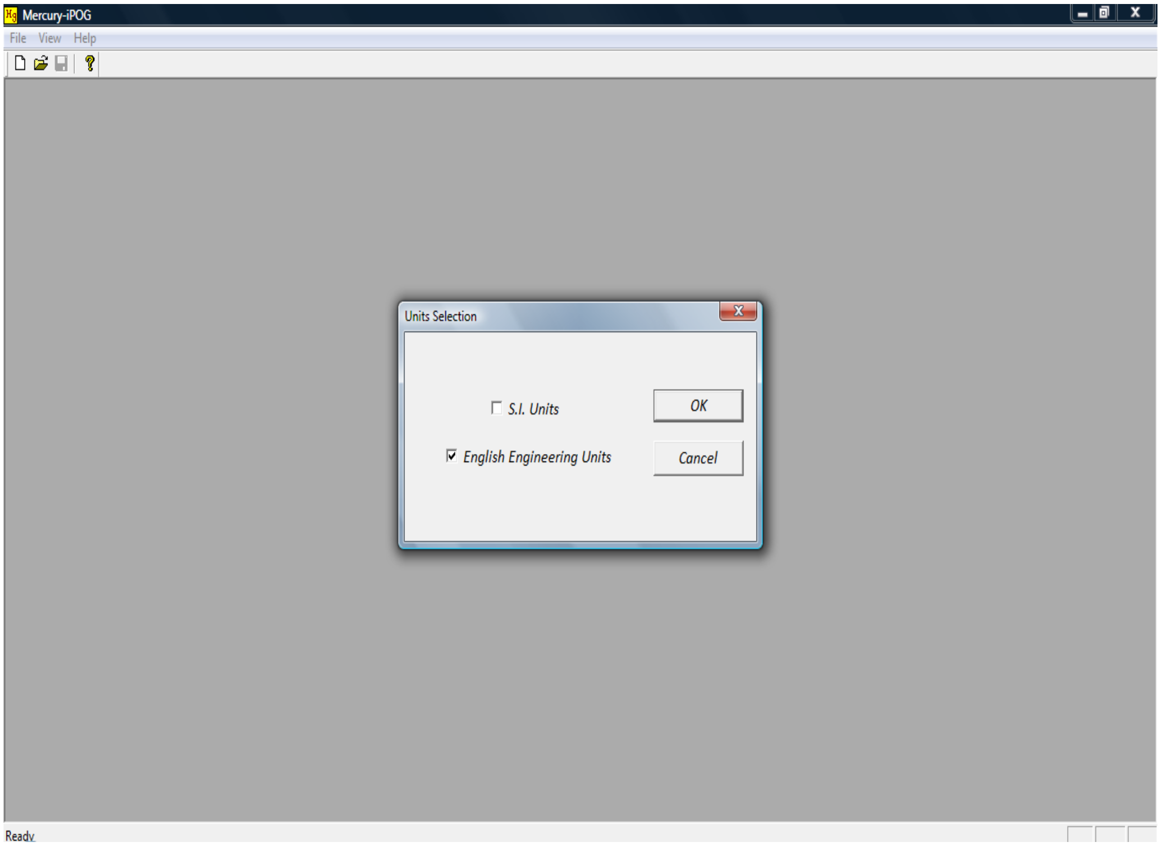


Figure 2-1.The ‘Parent’ window with superimposed ‘Units Selection’ window.

Enters Ctrl+N, or clicks the new file icon on the toolbar. This entry immediately brings up the ‘Units Selection’ window, which accepts the user’s preference on a system of units, either the International System of units (S. I.) or the English Engineering units.

From the ‘Parent’ window, users can also retrieve a session that had previously been saved in a custom format with an ‘.ipg’ file extension. This option starts under the ‘File’ menu with an entry of ‘Open’ or Ctrl+O, or with the open icon on the toolbar. That entry brings up the user’s file directory, so that the user can navigate to the location of the previously saved session records and select the one for the current session. This will be the most convenient way to set up cases that are similar to previous cases without having to complete every single stage of data entry. Once the GUI has been changed to the current case, it can be saved under the name of a new session record, as described below in the ‘Calculate’ section. These operations are identical to the standard file operations performed under a Windows operating system.

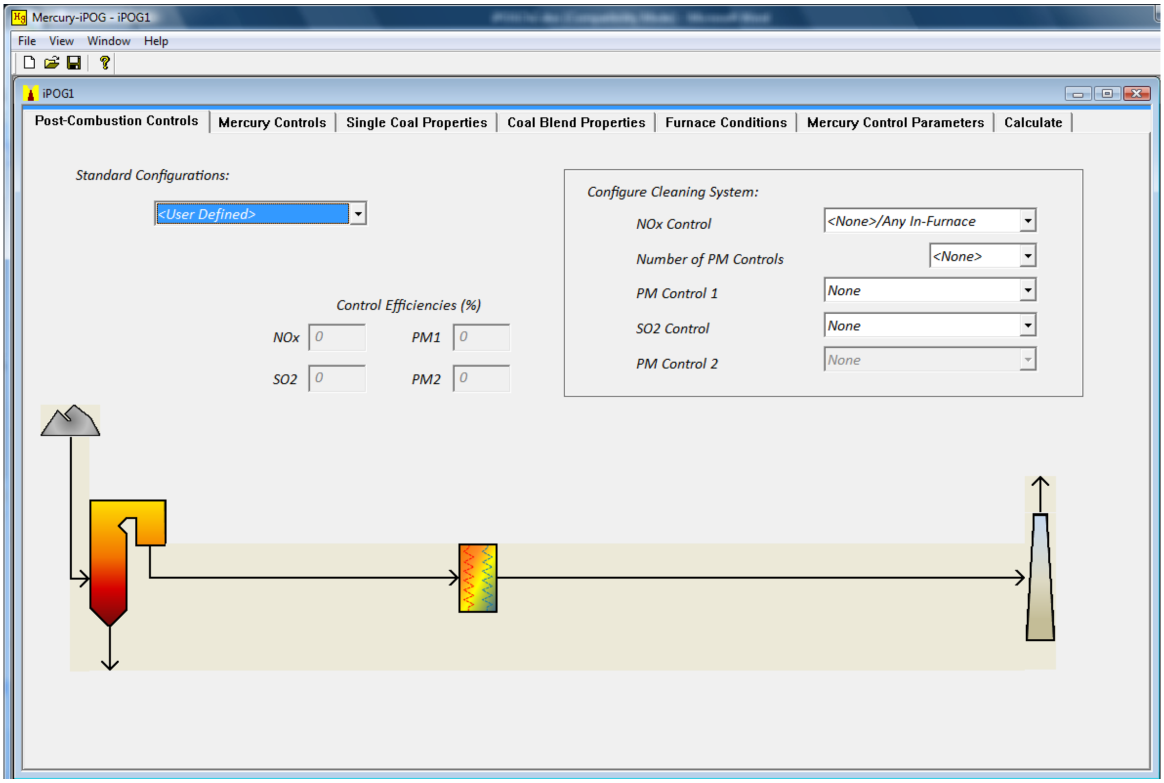


Figure 2-2.The first screen in a new session with the 'Parent' window.

Generic Screen Features

Once a user completes the 'Units Selection' window for a new session or retrieves a previous session, the user is presented with a new window with seven tabs within the 'Parent' window, as shown in Fig. 2-2. In new sessions, these tabs are used to navigate among the major steps in the sequence to enter all input specifications, to obtain the results for the test case, and to archive all entries. In retrieved sessions, these individual windows under the tabs are already populated with previous entries, so users need to select only those tabs with entries that need to be modified for parametric studies or for a different cleaning configuration.

When a particular tab is selected, it moves into the foreground along with its associated window to indicate the active topic. Six of the seven windows starting from the left accept inputs to describe the various operating parameters, while the final window on the right activates the calculation sequence and presents the results for Hg capture and emissions for the specified cleaning configuration. Default sets of input parameters are available in each input screen for ease of understanding and implementation. User-defined options can also be input in the same screens to allow expert users configure their systems in greater detail. Users can go back-and-forth among the first six input tabs to configure their test case and enter the input values in any order and to make any necessary adjustments.

The six tabs for data entry are labeled as (i)Post-Combustion Controls; (ii)Mercury Controls; (iii) Single Coal Properties; (iv) Coal Blend Properties; (v) Furnace Conditions; and (vi)Mercury Control Parameters. The execution tab is labeled as (vii) Calculate. The field of every screen contains four sections. The top bar contains the screen tabs. A section labeled ‘Standard Configuration’ and a register on the left side accepts blocks of default specifications from entry-level users. A larger box of registers to the right accepts detailed options from experienced users. The process schematic across the bottom is updated to show the subject cleaning configuration as new APCDs and Hg controls are added.

All data input registers are loaded in advance with default values, which would normally be altered by the user. This is done to ensure that at any stage the entry-level user can obtain a result by clicking on the ‘Calculate’ tab. However, in parametric case studies, this feature also admits the possibility that input specifications from one case may be inadvertently carried over in succeeding cases, as illustrated below. Some of the optional input values and configurations are restricted to allowable ranges so that every test case is represented in the Hg field-testing literature and compatible with commercial operating practices.

The normal sequence of input operations progresses from left to right through each window, except that the ‘Coal Blend Properties’ window is used only to implement a coal blend and the ‘Mercury Control Parameters’ window is used only if external Hg controls were specified in the ‘Mercury Controls’ window. Each of the iPOG™windows and the corresponding features are explained in detail in succeeding sections.

Post-Combustion Controls

The first step is to specify the APCD configuration by indicating controls for NO_X, PM and SO_2 emissions. iPOG™ users provide this information on the ‘Post-Combustion Controls’ window, which opens automatically once the user begins a session. This screenshot appears in Fig. 2-2. At the outset, no controls are selected so only the most basic flow diagram appears in which coal is fed into the furnace, and flue gas flows through an APH into the stack. The symbols and the color scheme used in the flow diagram were adapted from standard literature representations whereby devices operating at high temperatures appear in shades of red and yellow and units operating at lower temperatures appear in shades of blue.

The post-combustion pollution control equipment for NO_X, PM and SO_2 emissions control can be configured in two ways. Entry-level users use the menu of the most

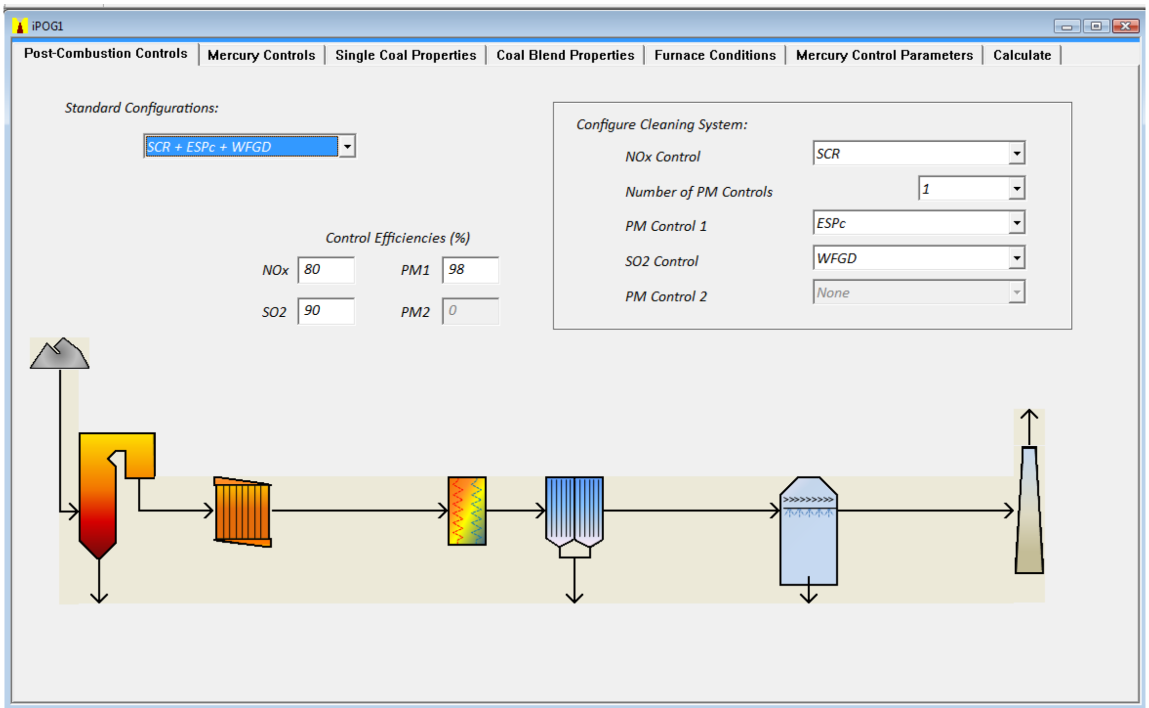


Figure 2-3. The 'Post-Combustion Controls' window for a default SCR+ESPc+WFGD cleaning configuration.

common configurations labeled 'Standard Configurations' on the left side of the screen. This menu covers the most popular cleaning configurations employed worldwide, including (i) ESPc-Only, (ii) FF-Only, (iii) ESPc+WFGD, and (iv) SCR+ESPc+WFGD. A fifth option labeled as (v) <User Defined> activates the block on the right for customized cleaning configurations. As soon as any of the first four items are selected, the process flow diagram is updated to the selected configuration. We believe that these standard configuration selections represent the vast majority of gas cleaning configurations installed on power plants worldwide, so even experienced users will often complete this screen with only the 'Standard Configurations' menu.

If the '<User Defined>' option is selected, the user must then specify the APCDs individually using the registers in the 'Configure Cleaning System' box on the right side of the screen. The configuration selection from the 'Standard Configurations' automatically populates the corresponding options on the right box. For example, if the user selects an SCR+ESPc+WFGD combination from the 'Standard Configurations' menu, the corresponding selections of APCDs appear in the right box along with the appropriate flow diagram, as shown in Fig. 2-3. In addition, three registers appear alongside the flow diagram with default values for the following performance indices: 'η_{NO} (%)', 'η_{PM} (%)', and 'η_{SO2} (%)'. These registers specify the NO_X reduction

Table 2.2.APCD Options for User-Defined Post-Combustion Controls.

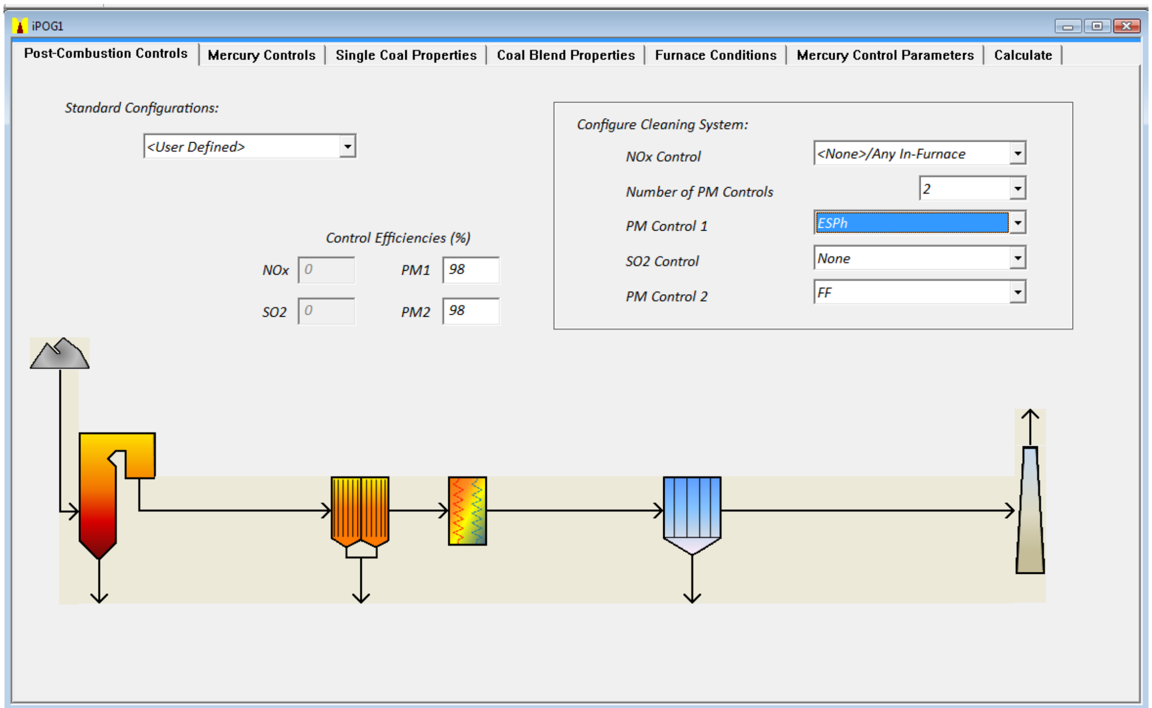
NO_x Control	Number of PM Controls	PM Control 1	SO_2 Control	PM Control 2
Any In-Furnace	None	None	None	None
SCR	1	ESPc	WFGD	ESPc
	2	ESPh	SDA	FF
		FF		
		Wet PM		

efficiency of the SCR, the PM capture efficiency of the ESPc, and the SO_2 capture efficiency of the WFGD, respectively. Whenever an APCD is selected on this screen, registers for the efficiency of that device appear automatically on the screen with default values. The default values in these registers can be overwritten by the user.

To specify configurations other than those in the Standard Configurations options, users may select values in the ‘Configure Cleaning System’ box on the right of the screen. The options under each drop-down menu are collected in Table 2.2. Specific forms of in-furnace NO_X control are not listed because the direct impact of low-NO_X burners, overfire air, SNCR, etc. on Hg emissions is minimal. But SCRs must be distinguished from the in-furnace NO_X controls, because SCR catalysts are often the most effective medium for Hg^0 oxidation in the system. The options for SO_2 control are none, WFGD, and SDA. For PM control, the iPOG™ supports none, ESPh, ESPc, FF, and Wet PM. It also permits up to two PM control devices in-series. This capability to configure multiple PM controls in-series is particularly important for users evaluating EPRI’s TOXECON™ technology for Hg control, whereby ACI is installed between an existing PM control device and an added pulse-jet FF; or into the trailing fields of an ESPc; or between two ESPc’s. Such PM control configurations must be initiated in this screen, then described further in the ‘Furnace Conditions’ and ‘Mercury Control Parameters’ windows.

When a user selects two PM controls, an additional drop-down menu to specify the second PM control device, labeled ‘PM Control 2,’ appears on the screen. Simultaneously, registers with default values for the PM collection efficiency of each device labeled ‘η_{PM1} (%)’ and ‘η_{PM2} (%)’ also appear on the screen, and these default efficiencies can be overwritten by the user. These features are evident in Fig. 2-4 where no NO_X or SO_2 controls were specified, and the gas cleaning systems have pairs of PM controls, the ESPh+FF and the ESPc+FF, respectively.

User-defined cleaning configurations can include any of the device combinations



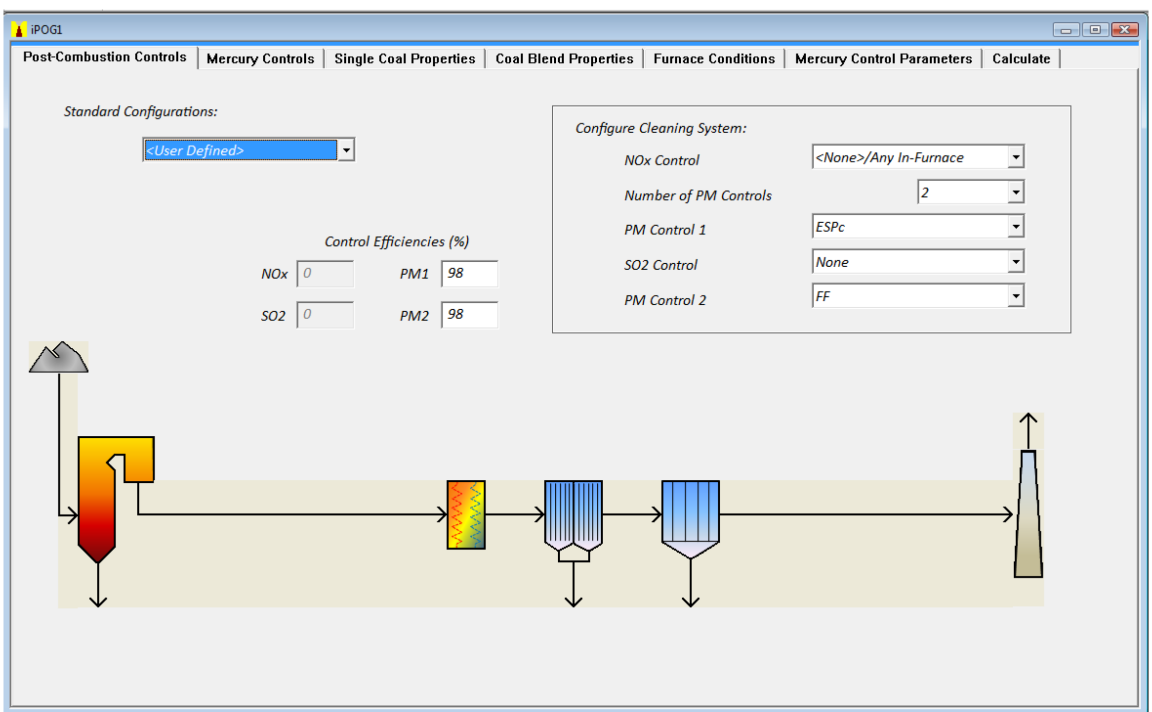


Figure 2-4. The 'Post-Combustion Controls' windows for user-specified configurations with (Top) ESPh+FF and (Bottom) ESPc+FF.

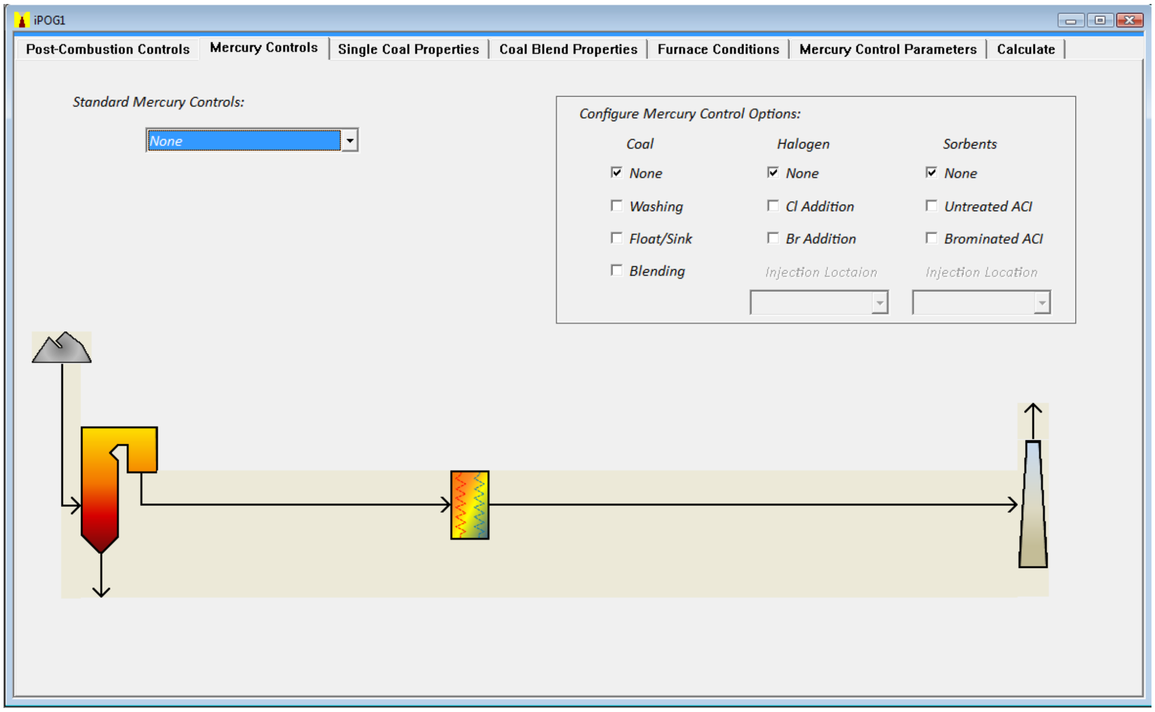


Figure 2-5. The 'Mercury Controls' windows for the configuration in Fig. 2-2.

in Table 2.2, within the following restrictions:

(i) Only one APCD option for NO_X and SO_2 control can be selected.

(ii) An SDA must precede a PM control device.

(iii) A Wet PM control, when selected, will be the only PM control.

(iv) Only ESPc and FF are available as selection options for the second PM Control.

(v) An integrated Wet PM and SO_2 scrubber unit must be input as the combination of Wet PM control and WFGD.

(vi) The efficiency of any APCD cannot be zero.

Mercury Controls

The next tab in the iPOG™ tabpage is 'Mercury Controls' and the corresponding screenshot appears in Fig. 2-5. Note that this screen is used only to configure the Hg controls, whereas the operating parameters for Hg controls such as ACI concentration and/or halogen loading are entered under the 'Mercury Control Parameters' tab. The

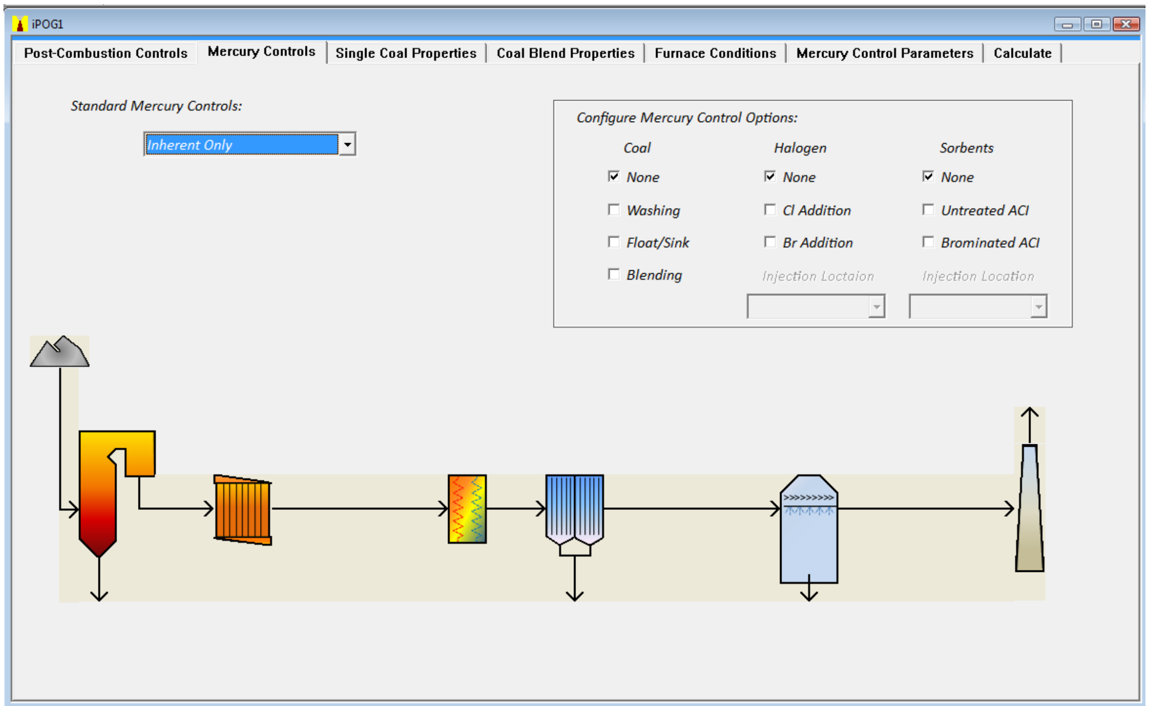


Figure 2-6. The 'Mercury Controls' windows for an SCR+ESPc+WFGD configuration.

screenshot corresponds to cases without any post-combustion control equipment, and was automatically carried over from the cleaning configuration in Fig. 2-2. Like the 'Post-Combustion Controls' screen, the 'Mercury Controls' screen is divided into two sections. The left section contains a single drop-down menu labeled 'Standard Mercury Controls' for selecting the most commonly used Hg control options. To evaluate more complex Hg control options, users would need to use the 'Configure Hg Controls Options' box on the right side. The 'Standard Mercury Controls' covers (i) Inherent Only, (ii) Untreated ACI, (iii) Cl Addition, and (iv) <User Defined>. 'Inherent Only' is the most common situation worldwide, whereas 'Untreated ACI' and 'Cl Addition' are the most common external controls in the USA.

The 'Inherent Only' option pertains to cleaning systems with APCDs for PM and/or SO_2 controls but no external Hg controls such as halogen addition or ACI. This selection is disabled and replaced by 'None' unless the plant contains at least one PM or SO_2 control device. Figure 2-6 shows the screen for the 'Inherent Only' selection for a case with an SCR+ESPc+WFGD combination. When the 'Inherent Only' option is selected on the left in Fig. 2-6, only the boxes labeled 'None' are selected for the different Hg control options on the right.

The second standard Hg control option, 'Untreated ACI,' refers to the injection of

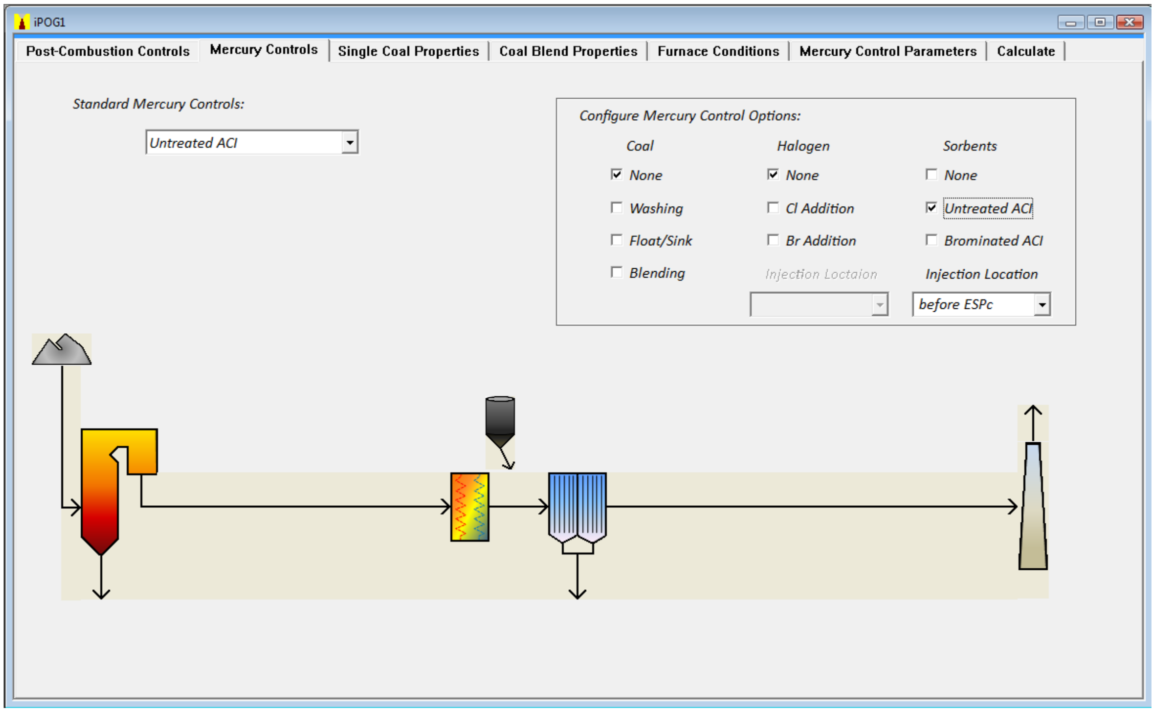


Figure 2-7. The 'Mercury Controls' windows for ACI into an ESPc.

a non-halogenated activated carbon sorbent upstream of the first PM control device. The cleaning system must therefore have at least one PM control device before this option can be activated. This option is, however, not supported for a Wet PM control or a combined Wet PM scrubber unit because we know of no field test data on such units in the Hg testing literature. The Hg control configuration screen for the 'Untreated ACI' option for a plant with ESPc-only appears in Fig. 2-7. When the 'Untreated ACI' option is selected from the standard Hg controls on the left, the 'Coal' and 'Halogen' options in the right box are disabled, so these checkboxes are labeled 'None.' Under the Sorbents menu, the checkbox labeled 'Untreated ACI' is selected, by default. In the flow diagram, the sorbent injection location is indicated by the icon for ACI immediately upstream of the first PM control, which is the ESPc in this case.

The third standard Hg control option, 'Cl Addition,' refers to a spray of $CaCl_2$ onto the coal as it is conveyed into the burners. This option is disabled unless the test case is configured with either PM or SO_2 control equipment. As with the screen for Post-Combustion Controls, selecting 'Cl Addition' under 'Standard Mercury Controls' automatically selects the corresponding choices in the 'Configure Mercury Controls Options' box on the right side. The 'Coal' and 'Sorbent' control options on the right would be disabled and labeled as 'None.' Under the 'Halogen' option, the 'Cl Addition' check box would be selected, and a lower menu for 'Injection Location' shows the 'In-

Table 2.3.User-Specified Options for Mercury Controls.

Coal	Halogen	Halogen Inj. Location	Sorbents	Sorbent Inj. Location
None	None	In-furnace/coal	None	before ESPh
Washing	Cl Addition	before SCR	Untreated ACI	before APH
Float/Sink	Br Addition	before ESPh	Brominated ACI	before ESPc
Blending		before APH		before FF
		before ESPc		before SDA
		before FF		within ESPh
		before SDA		within ESPc

furnace/coal' selection. The flow diagram would be updated with an icon indicating Cl addition onto the coal feed.

To activate Hg controls not listed under the Standard Hg Controls, users will select '<User Defined>' on the left drop-down menu, and then develop a custom control scheme in the 'Configure Mercury Control Options' box on the right. The iPOG™ allows experienced users to configure their custom controls under categories of (i) Coal, (ii) Halogen, and (iii) Sorbents, with the options under each category in Table 2.3.

The options under 'Coal' reduce the Hg entering the furnace by washing, float-and-sink, and blending. Any of these options may be selected for any gas cleaning configuration, and their icons will appear at the coal supply on the flow diagram. For the configuration in Fig. 2-5 without any APCDs, only the 'Coal' Hg control options are permitted. 'Washing' and 'Float/Sink' should only be applied to the properties of uncleaned, as-mined coals, for consistency with the database behind these estimates. Whereas 'Washing' and 'Float/Sink' can both be applied to the same set of coal properties, neither can be selected with 'Blending' unless the properties of all blend components will also be entered, rather than just the average properties of the blend. Thisis because it is impossible to back-calculate the properties of the blend components, such as S-contents, from the average blend properties.

The Hg control options under 'Halogen' cover halogen additions either to the coal before it is burned or into the furnace or into the flue gas ductwork downstream of the furnace exit. For no halogen addition, users select 'None'; otherwise, they select either Cl or Br addition and specify the injection location. Addition of both Cl and Br in the same test case is not supported because we know of no field tests with this form of Hg control. The injection location is specified in the drop-down menu labeled 'Injection

Location' under 'Halogen,' using one of the options in Table 2.3. Users can select either coal/in-furnace halogen injection or duct injection upstream of an APCD or the APH. Halogen addition before a Wet PM or WFGD is not supported. Among the allowable APCDs, only the ones specified in the screen for 'Post-Combustion Controls' appear in this menu, as expected. For example, for an SCR+ESPc+WFGD configuration, the user can indicate halogen addition on coal or in-furnace, before the SCR, before the APH, or before the ESPc. Only one addition location is permitted per calculation case.

The options for Hg control under 'Sorbents' allow users to configure ACI with either (i) Untreated activated carbon or (ii) Brominated activated carbon. Addition of both untreated and brominated ACI in the same test case is not supported. Sorbent injection is supported only for cases with PM controls and the injection location must be upstream of this equipment. The options for sorbent injection location are presented in Table 2.3. An example of 'Untreated ACI' was already shown in Fig. 2-7 and the 'Brominated ACI' option is configured in a similar manner. For the example in Fig. 2-7, the sorbent could be injected before the APH, before the ESPc, and within the ESPc (TOXECON-II™ configuration).

To specify Hg controls under multiple categories in a single calculation case, the user needs to simply select all the required control options on the right. For example, a test case for a ESPc-only cleaning configuration appears in Fig. 2-8 where both Cl addition and untreated ACI are selected as Hg control options. Since this configuration does not correspond to any standard Hg control option, the '<User Defined>' label appears on the left side under Standard Mercury Controls. On the right side, no options under 'Coal' are selected whereas 'Cl Addition' and 'Untreated ACI' are selected under 'Halogen' and 'Sorbent,' respectively. Chlorine was added to the coal feed, and untreated ACI was installed before the ESPc. After the injection locations were selected, the flow diagram was updated with the icons for Cl addition and ACI at their respective injection locations. Another example of user-defined Hg control options also appears in Fig. 2-8 corresponding to EPRI's TOXECON-I™ configuration. Here, untreated ACI is applied downstream of an ESPc and upstream of a FF. The ESPc+FF combination must be specified under the 'Post-Combustion Controls' tab and only the sorbent type and injection location need to be selected under the 'Mercury Controls' tab.

Whereas several Hg control options can be included in a single calculation case, the following restrictions will ensure that the resulting Hg control configuration is represented in the Hg field testing literature and is a commercially viable option: (i) The 'Inherent Only' option under 'Standard Hg Controls' cannot be selected with any other Hg control option under the 'Coal', 'Halogen' or 'Sorbent' categories, by definition; (ii)Both untreated ACI and brominated ACI cannot be selected simultaneously; (iii)If the gas cleaning system does not have PM controls, sorbent options are disabled; (iv)Both Cl addition and Br addition cannot be selected simultaneously; (v)If the gas cleaning system does not have PM or SO_2 controls, halogen injection options are disabled; (vi)Halogen

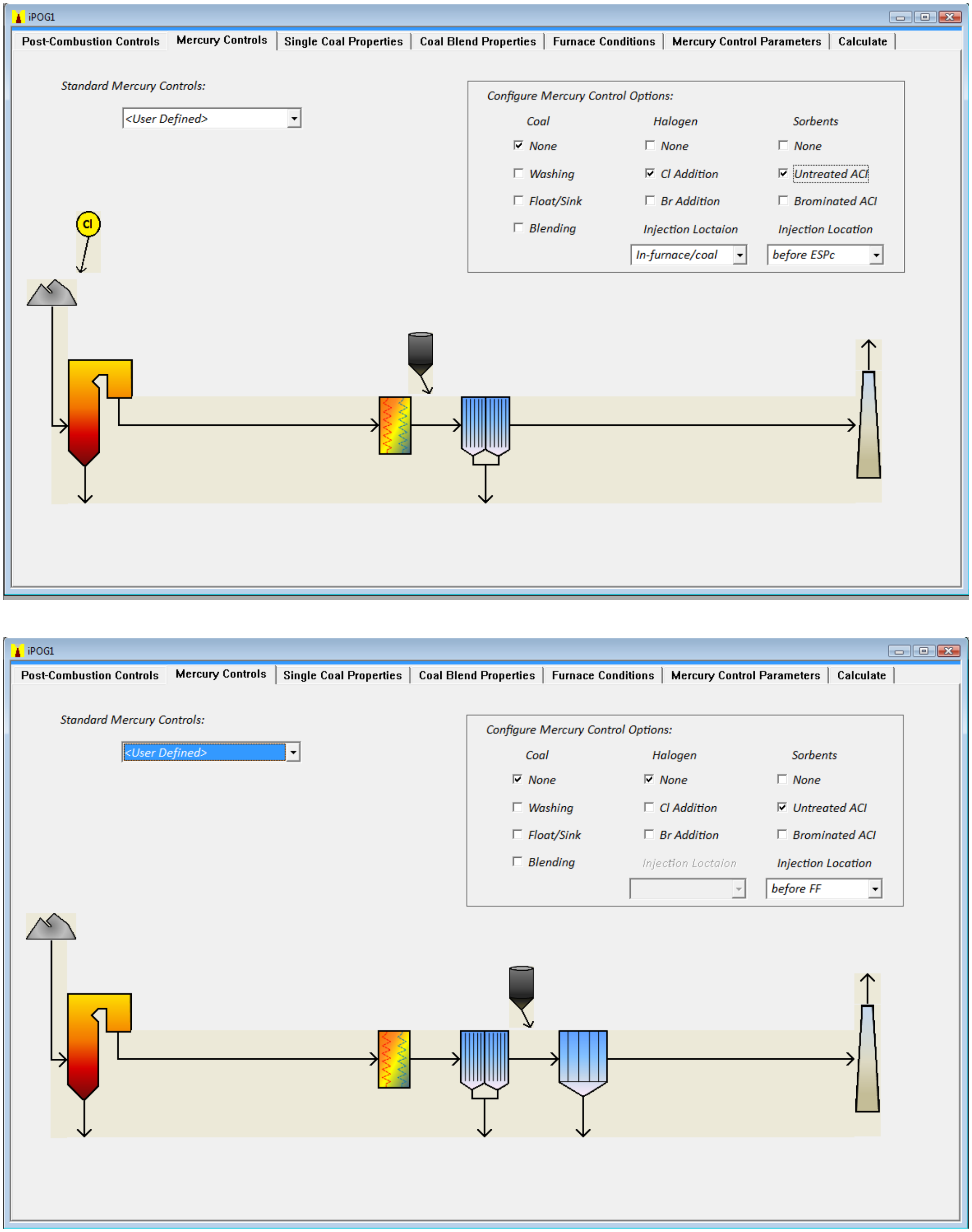


Figure 2-8. User-defined external Hg controls with (Top) Cl addition to coal plus ACI into an ESPc and (Bottom) EPRI's TOXECON I™ ACI scheme.

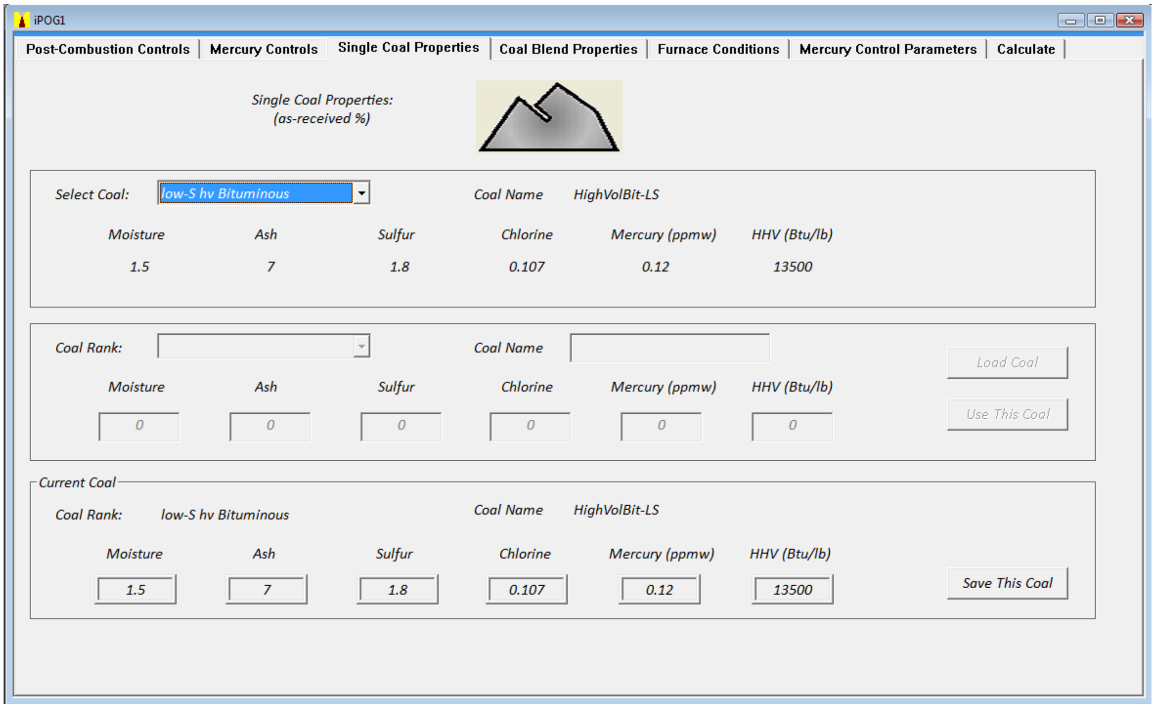


Figure 2-9. The 'Single Coal Properties' window with a default selection.

addition with 'Brominated ACI' is not supported; and (vii)Halogen addition before a Wet PM or a WFGD is not supported.

Single Coal Properties

After the cleaning system and Hg controls are configured, the third tab on the iPOG™ accepts the properties of individual coals. A screenshot appears in Fig. 2-9. The screen consists of three blocks, of which only two are active at a given time. Like the previous tabs on Post-Combustion and Hg Controls, the Coal Properties tab also contains default and user-defined options. The first horizontal block contains the Select Coal menu from which users can select one of the five standard sets of coal properties for (i) low-S high volatile (hv) bituminous; (ii) high-S hv bituminous; (iii) Anthracite, (iv) Subbituminous, and (v) Lignite. In addition, users can also select 'Blend' or 'User Defined' options under this menu. When one of the standard coals is selected, the coal label appears on the right followed by data registers for moisture, ash, sulfur, coal-Cl, coal-Hg, and the higher heating value (HHV). All coal properties are entered on an as-received basis, and the HHV is in Btu/lb or J/g. The entries in these registers for the five default coals cannot be altered unless the 'Coal Name' is also changed.

The horizontal block in the center of the window is used for specifying user-

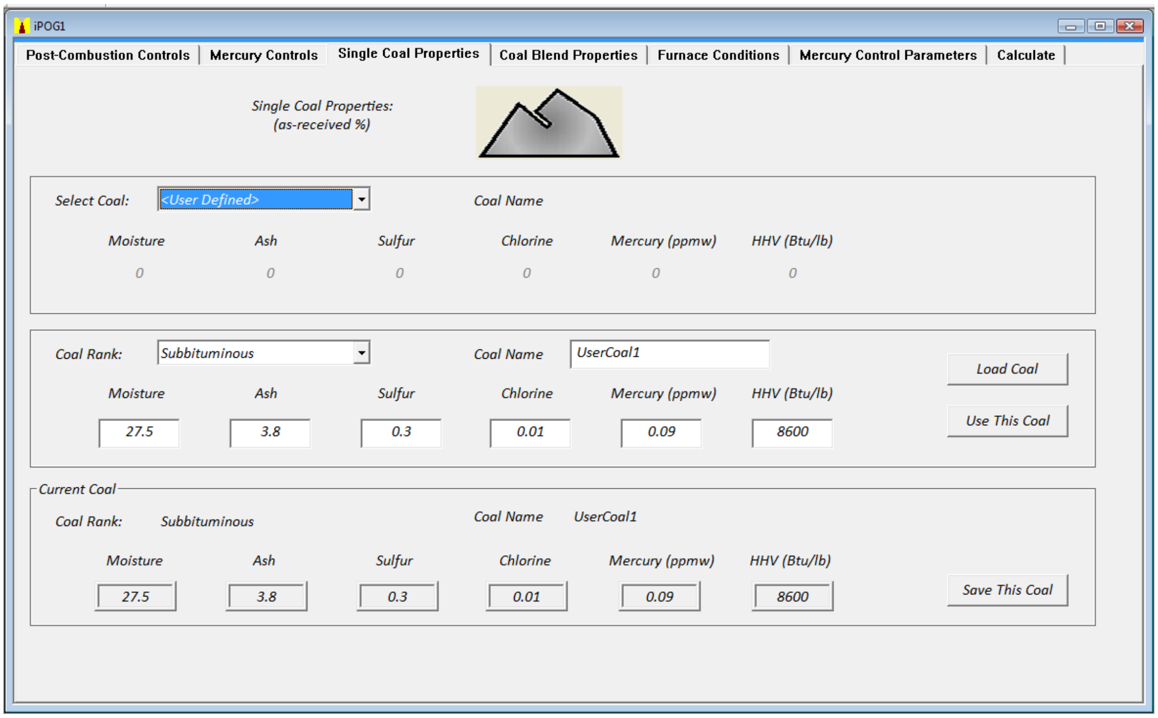


Figure 2-10. The ‘Single Coal Properties’ window with a user-defined selection.

defined coal properties and is disabled if one of the default coal properties is selected, as shown in Fig. 2-9.If the user needs to supply his or her own coal properties, then the ‘<User Defined>’ option must be selected from the ‘Select Coal’ menu, as seen in Fig. 2-10. Now the registers in the upper block are disabled while the second block is active. By default, the subbituminous rank is selected in the ‘Coal Rank’ menu. The user can select another coal rank from the drop-down menu and provide a label for the coal. If the user’s coal is medium- or low-volatile bituminous, it should be entered under either low- or high-S hv bituminous, depending on the S-content. This coarse assignment will not affect the accuracy of the results, by design. Note that the default entries for the selected rank automatically appear in the data registers. Users can then change whichever values they want, and leave any number of the default entries. This feature allows users to quickly change Hg and Cl contents in any particular coal sample, as often arises in parametric case studies.

Alternatively, users can quickly load any set of user-defined coal properties that were previously entered with the ‘Load Coal’ button. This action brings up a file directory from which the user can navigate to his file of coal properties that were previously stored in a MS Excel spreadsheet called ‘SaveCoal.csv’ under a user-defined label for the coal. This spreadsheet is in comma-delimited format, and should not be altered in any way by users. It can accommodate up to 15 sets of coal properties, excluding the five sets of default properties.

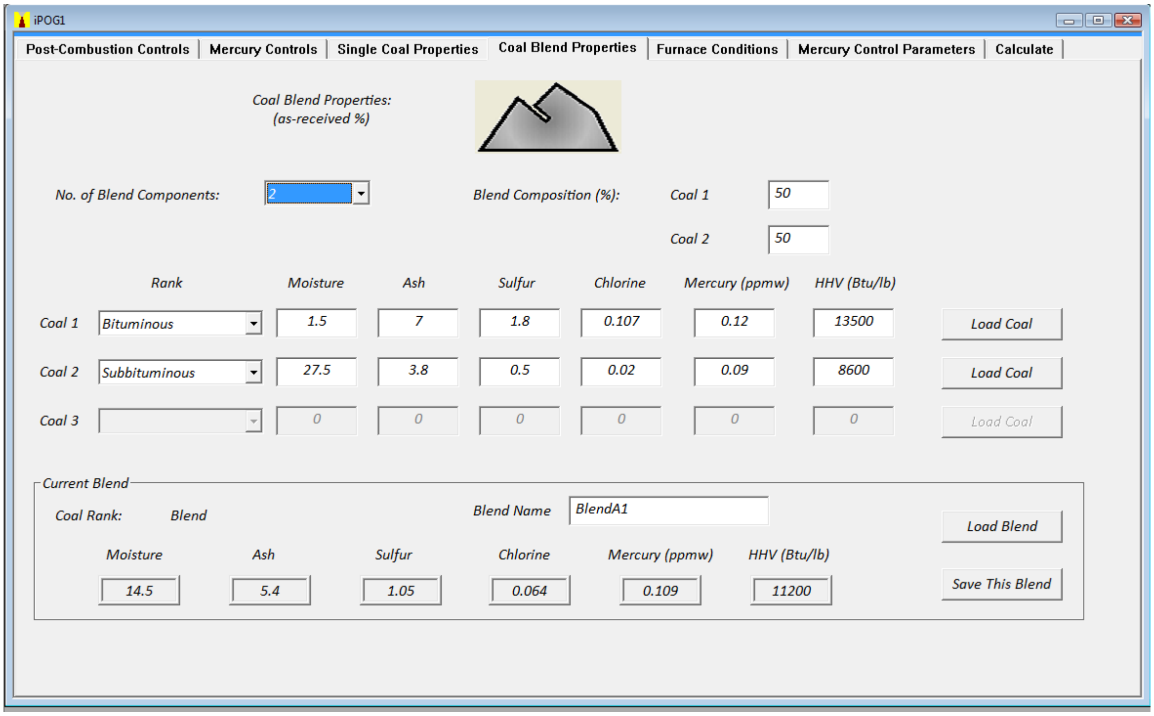


Figure 2-11. The 'Coal Blend Properties' window.

To apply the user-defined coal in the calculations, the user clicks the command button labeled 'Use this Coal,' which loads the properties into the bottom 'Current Coal' block. Whichever coal properties appear in the 'Current Coal' block can be saved in MS Excel spreadsheet format to the SaveCoal.csv file under the label entered in the 'Coal Name' register by clicking the 'Save this Coal' button. Once the properties have been saved this way, the properties are archived and can be retrieved into any succeeding calculation case using the 'Load Coal' button, provided that they are among the 15 most recent sets of saved properties.

Coal Blend Properties

To specify a coal blend, the Blend option is selected from the 'Select Coal' menu in the 'Single Coal Properties' window, which disables the rest of the blocks on this window. The coal blend properties can then be formulated in the 'Coal Blend Properties' window, as shown in Fig. 2-12. Users select either 2 or 3 blend components from the 'No. of Blend Components' register, and enter the component weight percentages into the registers for 'Blend Composition.' They then select the coal properties for the individual components among the default rank assignments; or load the desired coal rank and modify any of the individual properties to describe a new coal; or load previously entered sets of properties by using the 'Load Coal' button. The 'Load Coal' and 'Save This Blend' buttons work in the same way as for the single coal properties, except that blend

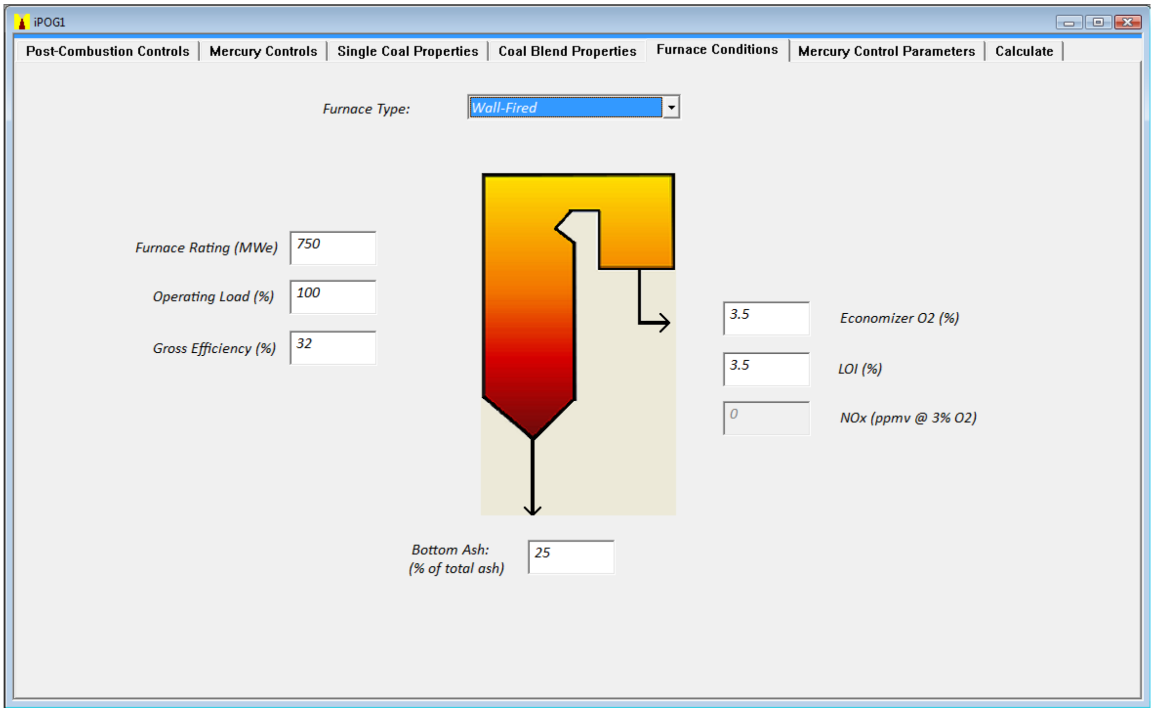


Figure 2-12. The ‘Furnace Conditions’ window.

properties are archived in a MS Excel spreadsheet called ‘SaveBlend.csv.’ Once a sample’s properties have been entered and saved under the Single Coal Properties tab, they can be retrieved into a coal blend without re-entering the properties. Similarly, the ‘Load Blend’ button in the bottom block can be used to retrieve the properties of any previously entered blend under a single name.

Furnace Conditions

The next tab in the iPOG™ titled ‘Furnace Conditions’ accepts the boiler operating parameters, as shown in Fig. 2-12. The only selection in this screen is the ‘Furnace Type’ menu, which appears at the top. Under this label, a user can select from (i) T-Fired, (ii) Wall-Fired, and (iii) Cyclone-Fired, where the default selection is a wall-fired furnace. Several input registers also appear on the screen pre-populated with sets of default values specific to each of the three furnace types, including (i) Furnace Rating in MW_e; (ii)Operating Load as a percentage of the rating; (iii)Gross energy conversion efficiency of the plant (η_{GROSS}) in %; (iv) Bottom Ash as % of total ash flow; (v)Economizer O_2 level in vol. %; (vi)Flyash LOI in wt. % of flyash from the first PM control device; and, perhaps, (vii)Economizer NO_X concentration in ppmv corrected to 3 % O_2.The NO_X concentration register is active only if the cleaning system contains a SCR.

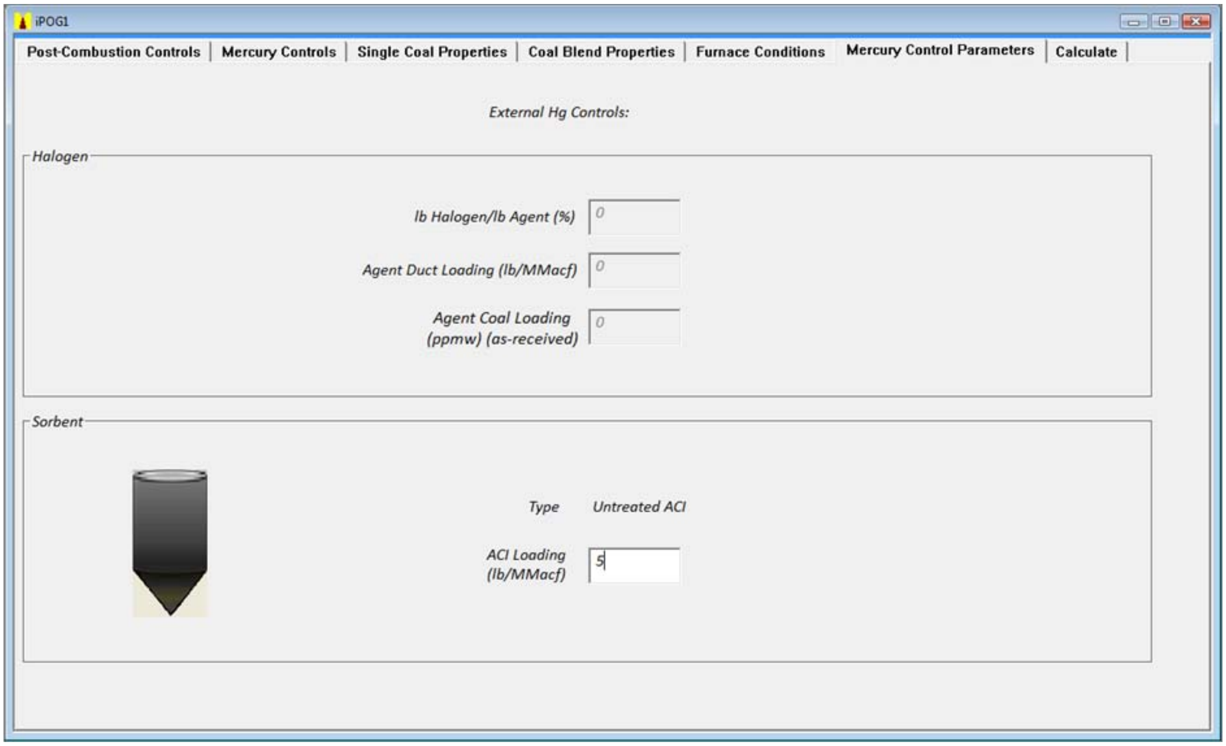
Table 2.4. Ranges of Acceptable Values for the Various Furnace Operating Conditions.

Operating Condition	Acceptable Range
Furnace Rating (MW_e)	25 − 2000
Operating load (%)	10 – 100
η_{GROSS} (%)	25 − 45
Economizer O_2 (%)	2.5 − 6
Bottom Ash (%)	10 − 80
LOI (wt. %)	0.2 − 15
NO_x (ppmv @ 3% O_2)	150 − 1500

Any of the input values on this screen can be changed by the user or left at their default specifications. However, they must be within reasonable bounds for commercial operations, which are collected in Table 2.4. None of these values can be zero. If the user enters values in the registers that are greater than or less than the acceptable range of values, then the respective highest or the lowest acceptable value will be indicated on the screen and used in the calculations.

Mercury Control Parameters

The next screen in the iPOG™ is titled ‘Mercury Control Parameters.’ It accepts operating conditions for the Hg controls configured previously under the ‘Mercury Controls’ tab. Specifically, this screen contains two blocks labeled ‘Halogen’ and ‘Sorbents’ which accept the injection concentrations for halogen and/or sorbent addition, respectively. The selections for either of these two blocks is active only if these controls were selected under the ‘Mercury Controls’ tab. The screen does not have any active selections if neither halogen nor sorbent injection was selected for Hg control, in which case it would simply be skipped. When ACI is the only Hg control option, as in Fig. 2-7 for an ESPc-only configuration, then the upper screen in Fig. 2-13 appears. Here the block for halogen addition is disabled and only the ‘Sorbents’ block is active. The sorbent type and injection location were already specified in the ‘Mercury Controls’ tab, so the label for sorbent Type has been carried over into this screen. Consequently, users need only enter the ACI loading in the units of pounds of sorbent per million actual cubic feet of flue gas (lb/MMacf) or grams per cubic meter (g/m^3) of actual flue gas.



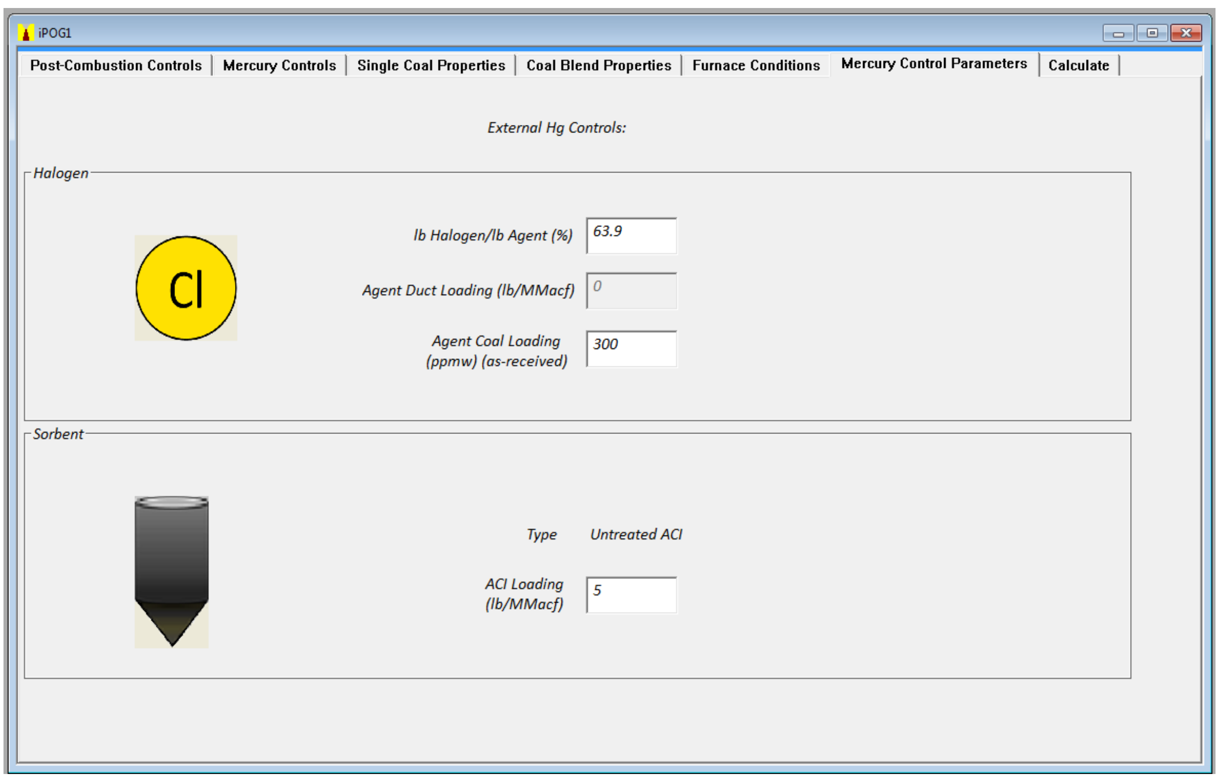


Figure 2-13. The 'Mercury Control Parameters' window for (Top) ACI into an ESPc and (Bottom) Cl addition on coal plus ACI into an ESPc.

If both halogen and sorbent additions were specified as Hg control options as, for example, in the upper panel of Fig. 2-8 for Cl addition and untreated ACI on an ESPc-only configuration, the lower screen in Fig. 2-13 appears. In the first block labeled ‘Halogen’, only the icon for Cl addition is active. Since several halogen additives are used commercially, the first input register labeled ‘lb Halogen/lb agent’ accepts the weight fraction of the halogen in the injected agent. For example, the most common Cl addition agent, $CaCl_2$, contains 63.9 wt. % Cl. This percentage is obtained by dividing the molecular weight of the total halogen by the molecular weight of the agent. The weight fractions of halogen in HCl and $Cl_2$are 97.3 and 100 %, respectively. Similarly, the weight fractions of halogen in HBr, Br_2 and $CaBr_2$ are 98.8, 100 and 80 %, respectively. The iPOG™ does not ask users to identify the injection agent but instead asks for the halogen content in the agent.

The next input value is the agent loading. Based on the agent injection location specified under the ‘Mercury Controls’ tab, one of the two boxes for agent loading becomes active. If, as in Fig. 2-8,the agent is injected into a furnace, either on coal or anywhere into the furnace firebox, then the register labeled ‘Agent Coal Loading’ becomes active. The user must enter the agent loading in ppmw of the coal on an as-received basis, as shown in Fig. 2-13. If the agent is injected at any location other than the furnace, then the register labeled ‘Agent Duct Loading’ becomes active and the user must enter the agent loading in lb/MMacf or g/m^3.

Users would complete this screen by entering the ACI loading in lb/MMacf or g/m^3. The input procedure is similar for Br addition or brominated ACI, except that halogen addition with brominated ACI is not supported.

Calculate

The final tab in the iPOG™ is titled ‘Calculate.’ Clicking on this tab activates the calculation sequence and fills the screen with the results as the Hg mass flows in the various input and output streams for the specified test case. The example in Fig. 2-14 describes a T-Fired furnace burning a low-S hv bituminous coal with a SCR+ESPc+WFGD cleaning combination without any sorbent or halogen injection for Hg control. Users should duplicate this case. The flow diagram for the specified configuration has now been supplemented with Hg mass flows in lb/h for all inlet and outlet streams. For each device that oxidizes or captures any Hg, the corresponding efficiency also appears with the outlet flowrate. In Fig. 2-14, the only Hg inlet stream is the coal feed and the outlet streams are the bottom ash, the ESPc ash, the WFGD blowdown, and the stack. The Hg capture efficiencies of the furnace ($\eta_{Hg,Furnace}$),ESPc ($\eta_{Hg,ESP}$) and WFGD ($\eta_{Hg,WFGD}$) are 0.5, 15.7 and 87.7 %, respectively. Since the plant also contains a SCR and WFGD, the Hg^0 oxidation efficiency across the SCR (${}^{SCR}X_{Hg}$) and the Hg^{2+} percentage into the WFGD also appear. The quantity ${}^{SCR}X_{Hg}$ is defined as follows:

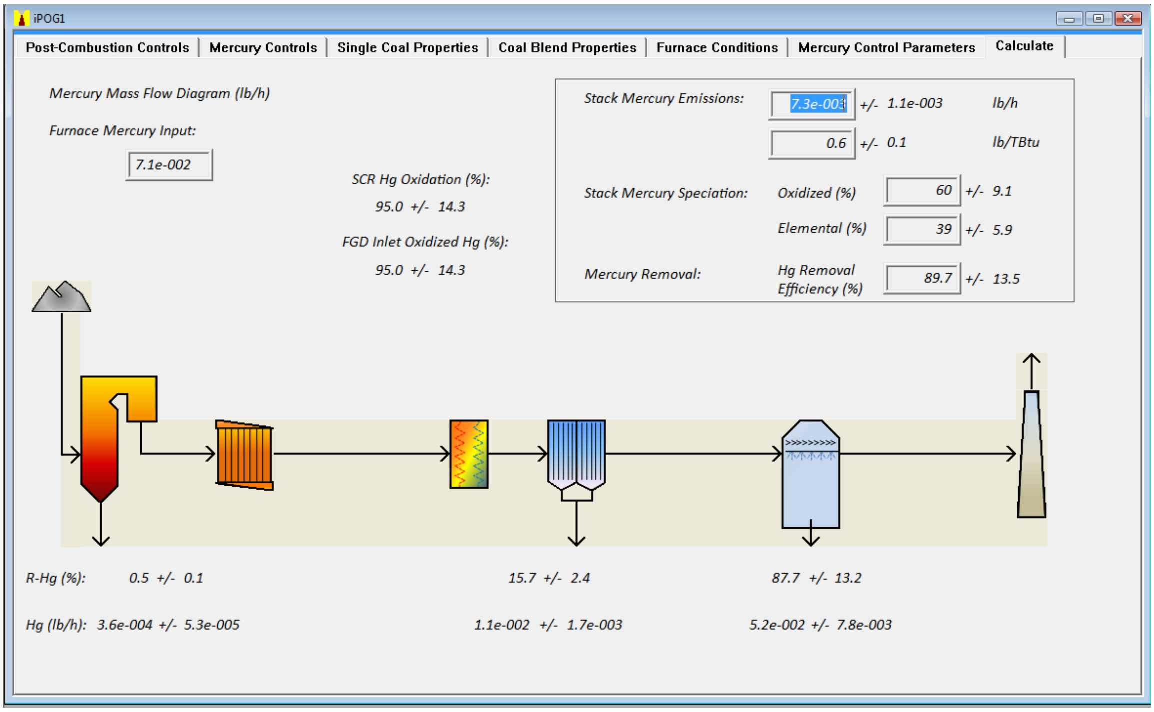


Figure 2-14. The ‘Calculate’ window for an SCR+ESPc+WFGD configuration.

$$ {}^{SCR}X_{Hg} = 100 \frac{C^{Inlet}_{Hg^0} - C^{Outlet}_{Hg^0}}{C^{Inlet}_{Hg^0}} \qquad 2.1 $$

where C^{Inlet}_{Hg0} and C^{Outlet}_{Hg0} represent the concentrations of Hg^0 vapor at the SCR inlet and outlet, respectively. Finally, the stack emissions of Hg in both lb/h and lb/10^{12}Btu appear in a summary block on the upper right corner of the screen. This block also reports the stack speciation of Hg and the overall Hg removal efficiency of the cleaning configuration.

A second output report in ASCII text format contains the results plus all the input entries, both default and user-defined. After each execution, this text report is issued in the resident directory under the name, ‘iPOG_Result.txt.’ It can be archived simply by changing the name before any other cases are executed.

The text file for the case in Fig. 2-14 appears in Fig. 2-15. Input values appear in the upper half, while the output from the ‘Calculate’ window appears under ‘Results.’ The furnace conditions are reported under the ‘Furnace Operating Conditions’ block, which is followed by the coal properties. This is followed by sections on the flue gas composition and the gas cleaning configuration, which lists each APCD and its performance efficiency. A section on Hg control would normally list the control technology and its operating conditions, except that this case had no external controls.

```
iPOG Output

Furnace Operating Conditions:
       Furnace Type   T-Fired
       Furnace Rating 750    MWe
       Operating Load 100    %
       Efficiency     32     %
       Bottom Ash     25     %
       LOI            3.5    %

Coal Properties (as-received):
       Single Coal    Y
       Blend          N
       Coal Rank      low-S hv Bituminous
       Coal Name      HighVolBit-LS

       Moisture       1.5    %
       Ash            7.0    %
       Sulfur         1.8    %
       Chlorine       0.107  %
       Mercury        0.120  ppmw
       HHV            13500  Btu/lb

Flue Gas Conditions:
       Economizer O2  4.5    %
       NOx            550    ppmv @ 3%O2

Gas Cleaning Configuration:                 Efficiency
       NOx Control    SCR    NOx Reduction  80     %
       PM Control     ESPc   PM Capture     98     %
       PM Control
       SO2 Control    WFGD   SO2 Capture    90     %
       PM Control

Hg Control:
       Coal:
                      None
       Halogen:
                      None
       Sorbent:
                      None

Results:
       SCR Hg Oxidation (%)          95.0   +/-    14.3
       FGD Inlet Oxidized Hg (%)     95.0   +/-    14.3
       Mercury Mass Flow:
       Input          lb/h
              Coal    7.11e-002
       Output         lb/h           +/-           Rem.(%) +/-
              Furnace 3.55e-004      5.3e-005      0.5     0.1
              ESPc    1.11e-002      1.7e-003      15.7    2.4
              WFGD    5.23e-002      7.8e-003      87.7    13.2
              Stack   7.33e-003      1.1e-003
       Stack Hg Emissions            +/-
              lb/h    7.33e-003      1.1e-003
              lb/TBtu 0.65           0.1

       Stack Hg Speciation           +/-
              % Hg2+  60             9.1
              % Hg0   39             5.9

       Total Hg Removal              +/-
              %       89.7           13.5
```

Figure 2-15. Version of 'iPOG_Results.txt' for the case in Fig. 2-14.

The results block gives the Hg conversions for the SCR and WFGD, followed by the Hg flowrates, the stack Hg emissions rates, and the stack Hg speciation. The final result lists the overall Hg removal for the entire cleaning system.

Archiving Sessions

Each session may be archived under a custom format denoted by the suffix '.ipg.' Users can save their sessions either by selecting the 'Save As…' item under the 'File' menu, or by clicking on the save icon in the toolbar. Either way brings up the file directory, which allows the user to navigate to the intended storage location and to enter a session-specific name for the session record. This record contains all the input and output for a particular calculation case, including all default and user-specified options.

Provided that these session records are present in the iPOG™ execution folder, they can be retrieved to quickly set up similar cases, or to repeat a calculation sequence for ranges of a single operating parameter. In the Parent Window, users will simply open the session records under the .ipg file name to pull up a complete series of screens that have been populated by the original entries. They can then change as many entries as necessary, execute the modified calculation sequence, and store the new session under a different name.

An Important Caution for Parametric Case Studies

Usually users will want to quickly run a series of calculation cases to understand how a particular process specification affects the Hg stack emissions. Perhaps the case study will focus on a series of different coals in the same cleaning system; or on implementing ACI on the same cleaning system for several different sorbent injection concentrations; or on the Hg removals from the same coal, furnace, and cleaning system for several different external Hg controls. Considering the large number of variables in our analysis, the possibilities are almost endless especially since, with some practice, users will be able to execute each calculation case literally in only tens of seconds.

Unfortunately, in programs like the iPOG™ that automatically populate all data entry registers with default values, there is a strong potential for inadvertently carrying over input from one case into the next, even when the user intends to have different values. This potential is particularly strong in the LOI specification, because LOI is determined by both the fuel characteristics and the furnace conditions. We can easily illustrate the hazard in the following case study. Suppose we want to evaluate the inherent Hg removals for all five of the default coal samples in an ESPc-only cleaning configuration fired by the same T-fired furnace. We begin a new iPOG™ session and select 'ESPc Only' under the 'Standard Configuration' menu on the 'Post-Combustion Controls' window. We need not enter anything on the 'Mercury Controls' window, because this case has no external Hg controls. We then select the low-S hv bituminous

Table 2.5.Incorrect and correct total Hg removals for inherent control of an ESPc-only configuration for the five default coals.

Coal	Incorrect	Correct
Lignite	13.1	9.7
Subbituminous	21.2	11.8
Low-S hv bituminous	16.1	16.1
High-S hv bituminous	14.2	14.2
Anthracite	21.1	31.4

sample from the 'Select Coal' menu on the 'Single Coal Properties' window. We may skip the blending window, and select 'T-Fired' for the Furnace Type on the 'Furnace Conditions' window. We can then skip the 'Mercury Control Parameters' window, and execute the first case in the 'Calculate' window. We record the Hg removal efficiency as 16.1 %. For the next case, we simply select another coal from the 'Select Coal' menu on the 'Single Coal Properties' window, and then select the 'Calculate' window to view the removal efficiency for the new coal. The last step is repeated to cycle through all the remaining coal samples.

Users should verify that this procedure gives the results labeled as 'Incorrect' in Table 2.5; in fact, those familiar with Hg emissions control will immediately recognize a problem because more Hg is removed with the low-Cl subbituminous coal than with all three coals of higher rank, which would be very unusual for an ESPc-only cleaning configuration.

This problem was caused by a failure to re-set the input to the correct default LOI values when each new coal was selected. Consequently, all cases were evaluated with the default LOI of 3.5 wt. %, which happens to be correct for both hv bituminous coals, but not for the other three. To reset this crucial input entry, we need to change the specification on Furnace Type in the 'Furnace Conditions' window to either 'Wall-Fired' or 'Cyclone-Fired,' and then re-set it to 'T-Fired' every time a new set of coal properties is entered. Users should verify that this procedure does, indeed, load the proper default LOI specification for each of the five default coals. Then we obtain the correct results in Table 2.5, which exhibit the expected tendency for greater Hg removals for coals of progressively higher rank.

Since LOI is determined by both the furnace firing conditions as well as the fuel properties, there was no way to eliminate the potential for this error in the window design. Users will have to resist the tendency to flash though only those screens that they intend to change while ignoring all others, and review each screen with active input before any new calculation case is executed.

3

TUTORIAL

Overview

This chapter provides a comprehensive review of the previous two chapters by demonstrating various applications of the iPOG™. Four case studies are worked out in detail. The tutorial begins with a case that illustrates the most basic considerations of how coal-Cl, LOI, and furnace load affect the Hg emissions from a simple ESP-only gas cleaning system. The second case evaluates the most important effects of adding an SCR to a cleaning system, including emissions estimates with the SCR in-service, out-of-service, and bypassed. Next we evaluate long-term Hg control strategies based on ACI only, and ACI with FGD. The fourth case illustrates how the iPOG™ can be used to obtain the same Hg emissions performance with a subbituminous coal and a subbituminous/bituminous blend as with an Eastern bituminous, via injection of a chlorination agent with and without ACI.

Follow along on your computer as we set up the input spreadsheets and review the output for each case or, better yet, apply the same steps to fuels and cleaning conditions that have your more immediate interest. Just be sure to realize that most of the trends in these cases should not be generalized to other fuels and gas cleaning conditions. Observations such as, "Only reductions in coal-Cl affect Hg emissions" and "The SCR oxidized essentially all the Hg^0 at its inlet" do not apply to many common flue gas cleaning situations. With iPOG™, you do not need to rely on these tendencies anyway, because the calculations are so simple to set up and execute. When in doubt, just run the calculations to characterize the Hg transformation behavior for your particular gas cleaning conditions.

Prerequisites

Anyone proceeding through these cases should know how to:

1. Load a new session from an existing session record.
2. Create a new session.
3. Change entries in an existing session record.

4. Execute iPOG™.
5. Locate and display the calculation results.

Case 1.Assess the Most Important Uncontrolled Variations in Hg Emissions from an ESP-Only Cleaning System

Case 1, Description

Your responsibilities include managing the Hg emissions from a 35 MW_e wall-fired process furnace firing low-S bituminous coal with an ESP-only cleaning system. Since the Hg emissions from this furnace will probably remain uncontrolled for the foreseeable future, your primary interest is to estimate the range of variation in the Hg emissions under normal operation. Only coal from a single mine is fired at this furnace. A typical LOI value is 9 wt %, and the economizer O_2 at full load is 3.1 %.

Case 1, Approach

In this simple gas cleaning system, the only means to remove Hg from the flue gas is as HgP on the flyash recovered by the ESP. In turn, the HgP levels will be governed by the levels of coal-Cl and LOI. Since the fuel supply will remain very stable, no other property variations need to be considered. The only other operating condition that could affect Hg emissions is the diurnal variation in the furnace load. As a starting point, we will use iPOG™ to assess how the largest expected variations in coal-Cl, LOI, and furnace load affect the Hg emissions.

Case 1, Method

To define this simple gas cleaning system, perform the following steps: Initiate a new iPOG™ session; in the ‘Post-Combustion Controls’ window, select the ‘ESP Only’ option from the standard configurations; and in the ‘Mercury Controls’ window, select the ‘Inherent Only’ option from the standard mercury controls. For the sake of illustration, select the default ‘low-S hv Bituminous’ to define the fuel in the ‘Single Coal Properties’ window. Since only a single coal is used, the ‘Coal Blend Properties’ window can be skipped. Next, select the ‘Wall-Fired’ furnace type in the ‘Furnace Conditions’ window to load the default set of parameters. Since the plant in this example is rated at 35 MWe, modify the furnace rating accordingly. Enter an LOI of 9 wt. % and an economizer $O_2$of 3.1 %. This completes all the input data specifications for the present case since there are no external Hg control parameters that need to be specified in the ‘Mercury Control Parameters’ window. Execute the case by clicking the ‘Calculate’ window. The removals, mass flow and stack emissions are calculated and displayed in the window and the detailed results can be archived by re-naming the 'iPOG_Result.txt'or by saving the session in .ipg format. For this case, the predicted stack Hg emission rate is 4.5 lb/TBtu, which represents removal of 34.5 % Hg as HgP.

To examine the effect of Cl variations, the user needs to alter the coal-Cl levels while keeping everything else the same. We examine coal-Cl levels from 0.027 to 0.053 wt. % vs. the default value of 0.107 wt. %. To setup these cases: (i) Select the '<User Defined>' option in the 'Select Coal' register on the 'Single Coal Properties' window; (ii) Select the 'Bituminous' option under coal rank and modify the coal-Cl as needed; and (iii) Click on the 'Use This Coal' button to apply the modified values to the current calculation case. Examine the 'Furnace Conditions' window to ensure that the intended LOI and furnace values are loaded and proceed to the 'Calculate' window.

To examine the effect of LOI variations, select the default coal properties of the 'low-S hv Bituminous' coal without any changes. Then change the LOI value in the 'Furnace Controls' window as required and proceed to the 'Calculate' window. Examine LOI at 13.5 and 4.5 wt. % vs. the default value of 9 wt. %. The results from the Cl and LOI parametric test cases are shown in Table 3.1.

Table 3.1.Impact of coal-Cl and flyash LOI variations for a bituminous coal in an ESP-only configuration.

Case	Coal-Cl ar wt. %	LOI wt. %	Hg Emissions lb/TBtu	Hg Removal %	Stack Hg^{2+} %
ESPOnly	0.107	9.0	4.5	34.5	85
	0.053	9.0	4.5	35.0	56
	0.027	9.0	4.4	35.2	42
	0.107	13.5	3.6	48.0	93
	0.107	4.5	5.4	20.9	76

Our study of load variations is based on cases with 100, 90, 75, and 60 % of the furnace rating. For this series, we suppose that the economizer O_2 increases from 3.1 to 3.4 to 4.2 to 4.6 % while the LOI diminishes from 9 to 8 to 6.5 to 5.5 wt. % over the four load levels. We examine all these cases for the default 'low-S hv Bituminous' coal with all other parameters unchanged. Consequently, all changes will be made only on the 'Furnace Controls' window. For each case, the desired operating load and the corresponding economizer O_2 and LOI are entered before proceeding to the 'Calculate' window. Execute the three cases for reduced loads to obtain the results in Table 3.2.

Case 1, Discussion

When coal−Cl was varied by a factor of four at an LOI of 9 wt. %, the Hg removal was hardly perturbed. The fraction of Hg^{2+} exiting the ESP, however, increased from 42 to 85 % with the quadrupling of Cl. This behavior would have significant implications

Table 3.2.Impact of load variations for a bituminous coal in an ESP only configuration.

Load, %	Econ O_2, %	LOI, wt.%	Hg Emissions lb/TBtu	Hg Removal %	Stack Hg^{2+} %
100	3.1	9.0	4.5	34.5	85
90	3.4	8.0	4.6	31.1	83
75	4.2	6.5	4.7	26.2	81
60	4.6	5.5	4.8	22.8	79

regarding capture of Hg^{2+} exiting the ESP if scrubber systems are installed downstream. The ± 50 % variations in LOI changed the Hg removals to 48.0 and 20.9 %,respectively, so that Hg removals increased in near-proportion to the LOI levels. Mercury removals diminished for progressively lower furnace loads, due primarily to the lower LOI levels associated with the reductions in load. So the key to maintaining the inherent Hg control at this plant will be to ensure that LOI levels do not fall substantially below their baseline values.

Case 1, Extensions

Review the results for all parametric cases to estimate the inherent Hg control benefits of adding an FGD. Since the Cl and LOI levels and consequently the Hg^{2+} at the stack are high, a majority of the Hg^{2+} can be expected to be captured in the FGD.

Case 2. Develop a Strategy to Manage the Impact of Adding an SCR to an ESP-Only Cleaning System

Case 2, Description

The gas cleaning system in one of your company's large baseload plants firing bituminous coal is being expanded with a new SCR and FGD. You have been asked to assess the impact on Hg emissions in three operating scenarios: (1) full-SCR operation during the ozone season; (2) out-of-service SCR operation (with no NH_3 injection); and bypassed SCR. You should also consider how the Hg emissions would be affected if the FGD is taken out of service during any of the three SCR scenarios.

Case 2, Approach

On the premise that the bituminous coal fired in this furnace is a high-S bituminous, we can reasonably expect the fuel to also contain sufficient Cl to retain a majority of the Hg^{2+} in the FGD. Consequently, we need to simulate the complete SCR/ESP/FGD combination with and without NO reduction, and a single case with no SCR.

Case 2, Method

To define this gas cleaning system, select the 'SCR+ESP+WFGD' option from the standard configurations in the 'Post-Combustion Controls' window, and in the 'Mercury Controls' window, select the 'Inherent Only' option from the standard mercury controls. For the sake of illustration, select the default 'High-S hv Bituminous' to define the fuel in the 'Single Coal Properties' window. Since only a single coal is used, the 'Coal Blend Properties' window can be skipped. Next, select the 'Wall-Fired' furnace type in the 'Furnace Conditions' window to load the default furnace parameters. We assume that the default properties in this window are applicable to this plant. This completes all the input data specifications. Execute the case by clicking on the 'Calculate' window. For this test case, the predicted stack Hg emission rate is 1.5 lb/TBtu, which represents an overall removal of 83.9 % Hg, of which approximately 82 % was removed in the WFGD and 18 % in the ESPc.

To evaluate the out-of-service SCR, enter a value of 10 for the NO reduction efficiency (%) in the "Post-Combustion Controls" window, since 10 % is the minimum value supported. Retaining all other values, we find that the predicted overall Hg removal increased to 86.8 %. A slightly higher removal could be expected for an out-of-service SCR, because NH_3 inhibits the chlorination of the SCR catalyst which diminishes the Hg^0 oxidation rate. But the difference in the removals in this case would be within the margin of uncertainty.

For a case without an SCR, the user can select the 'ESP+WFGD' option from the standard configurations in the 'Post-Combustion Controls' window. Since none of the other properties are changed, the case is ready for execution. When the SCR is removed, the total Hg removal falls dramatically to 49 % from 83.9 % due to the much lower fraction of Hg^{2+} entering the WFGD.

Case 2, Discussion

In summary, during the ozone season we expect the inherent Hg control to exceed 80 % of the Hg inventory. Otherwise, the Hg removal approaches 90 % if flue gas passes through the SCR without NH_3 injection, but falls to less than 50 % if the SCR is taken out of service. The satisfactory baseline performance is due to the moderately high Cl-content of this bituminous coal. The associated HCl concentration is about double the threshold where a Cl deficiency inhibits Hg^0 oxidation across the SCR. Notwithstanding, the case without NH_3 injection gave a removal approaching 90 %, due to the elimination of the competitive interference of NH_3 adsorption on HCl adsorption along the SCR catalyst. In other words, the surface coverage of HCl is significantly higher without NH_3 injection, as expected, and the Hg removal increases accordingly. But the Hg removal plummeted when the SCR was eliminated from the gas cleaning system. If the penalties for Hg emissions were high enough, it could conceivably be prudent to pass flue gas through the SCR year-round.

Case 2, Extensions

Assess the impact of an SCR for coals with different coal-Cl levels. In addition, consider how the Hg emissions would be affected if the FGD is taken out of service during any of the three SCR scenarios by simulating SCR+ESP and ESP only configurations.

Case 3. Determine Which Hg Control Strategy is Most Susceptible to Variations in Coal-Cl: ACI Into an ESP or an ESP/FGD Combination

Case 3, Description

State regulations require 90 % Hg controls on one of your company's plants within two years. Since this plant normally operates on a variety of hv bituminous coals from various sources, the coal-Cl levels are highly variable. You have been asked to estimate how these Cl-variations will affect conventional ACI as well as addition of FGD.

Case 3, Approach

We first need to establish the range of the coal-Cl variation which, for sake of illustration, is taken as 0.010 to 0.100 ar wt. % in the coal. We then run cases across this range for (1) ACI at an injection rate sufficient to achieve the ultimate, asymptotic Hg removal with an ESP Only and (2) an ESP/FGD combination.

Case 3, Method

We first examine the effect of Cl variations on the Hg removal by ACI for an ESP only configuration. First, select the 'ESP Only' option from the standard configurations in the 'Post-Combustion Controls' window. Then specify ACI in the 'Mercury Controls' window by selecting the 'Untreated ACI' option under the 'Standard Mercury Controls' on the left of the screen or by checking the box under Sorbents in the box on the right side. Either selection defines untreated ACI before the ESP, which is suitable to this case. For the sake of illustration, the fuel properties for this application pertain to the default 'High-S hv Bituminous' coal, except that the coal-Cl levels will be set to 0.01, 0.05, and 0.10 ar wt. %. The coal-Cl variations for this case are implemented as described in Case 1. The user then selects the 'Furnace Conditions' window to load the "Wall-Fired" furnace type and the associated default set of parameters. We assume that the default properties in this window apply to this plant. Next navigate to the 'Mercury Control Parameters' window to define the untreated ACI concentration. On activating the tab, the untreated ACI option appears with an injection concentration of 5 lb/MMacf. We increase this value to 7 lb/MMacf to ensure asymptotic performance and run the calculation for the three different coal-Cl values.

For the second series, select the 'ESP+WFGD' option from the standard configurations in the 'Post-Combustion Controls' window and follows the procedure outlined above for the ESP-Only case to examine the effect of Cl variations on the capture of Hg by ACI. The results are summarized in Table 3.3:

Table 3.3. Impact of coal-Cl variations on Hg removals for ACI into an ESPc and into an ESPc+WFGD configuration.

Case	Coal-Cl ar wt.%	Hg Emissions lb/TBtu	Hg Removal %
ACI Only	0.010	2.4	63.5
	0.050	1.6	76.8
	0.100	0.4	93.5
ACI w/FGD	0.010	1.9	72.1
	0.050	1.2	82.7
	0.100	0.3	95.3

Case 3, Discussion

The variation in coal-Cl significantly affects Hg removals in both the ESP-only and ESP+WFGD configurations. For an ACI concentration of 7 lb/MMacf, the Hg removal increased from approximately 64 to 94 % when coal-Cl was increased from 0.01 to 0.10 ar wt. %. Hg removals for ACI into an ESP+WFGD configuration were consistently higher than the ESP-only system and the removals reached an asymptotic saturation sooner than the ESP-only system. But the asymptotic Hg removals were very similar, so both approaches could be viable. Bear in mind that the lowest Cl-content in this example is below the typical lower limit for hv bituminous coals, so the results for the intermediate and high Cl level are more realistic. The ESP recoveries are substantial in all cases due to the elevated LOI level; in fact, this contribution represents almost 40 % of the ESP recoveries in the cases with ACI. Conversely, the FGD retention were modest because no SCR was present to oxidize most of the Hg^0 vapor.

Case 3, Extensions

Perform additional sensitivity studies to characterize variations in LOI (from 2 to 10 wt. %), and optimize the ACI concentration for the two configurations.

Case 4. Figure Out How to Achieve the Hg Removals for an Eastern Bituminous With a Subbituminous/Bituminous Blend and a Subbituminous Coal Through a SCR/ESP/FGD

Case 4, Description

Your company has been converting its large baseload plants to operate on subbituminous coals from the Powder River Basin (PRB) in blends and as straight fuels. The plant you manage already added a SCR/ESP/FGD combination, and will soon be regulated for Hg emissions by the state. Use iPOG™ to generalize the Hg speciation data you have for a bituminous coal to devise a strategy to maintain the same Hg removal with PRB and a 50:50 PRB/bituminous blend.

Case 4, Approach

Since this cleaning system contains SCR and FGD, we will utilize oxidation of Hg^0 across the SCR and retention of Hg^{2+} in the FGD to meet the goals of this project. We may not need to compensate for the reduction in LOI with PRB co-firing and direct firing (by adding ACI, for example), although the lower LOI values should be entered into our calculations. Instead, we will compensate for the lower HCl concentrations in the flue gas by injecting $CaCl_2$ into the furnace whenever PRB is fired. Hence, this case determines how much $CaCl_2$ is needed to match the target Hg removals with the blended and whole PRB fuels.

Case 4, Method

First, we determine the inherent Hg removal for an Eastern bituminous coal. To define this gas cleaning system, select the 'SCR+ESP+WFGD' option from the standard configurations in the 'Post-Combustion Controls' window, and in the 'Mercury Controls' window, select the 'Inherent Only' option from the 'Standard Mercury Controls.' For the sake of illustration, select the default 'High-S hvBituminous' to define the fuel in the 'Single Coal Properties' window. Since only a single coal is used at first, the 'Coal Blend Properties' window can be skipped. Next select the 'Wall-Fired' furnace type in the 'Furnace Conditions' window to load the default set of parameters. We assume that the default properties in this window apply to this plant. This completes all the input data specifications for the bituminous coal. Execute the case by clicking on the 'Calculate' window. The predicted stack Hg emission rate is 1.5 lb/TBtu, which represents an overall removal of 83.9 % Hg. Next, we evaluate the inherent removal for the subbituminous coal. Change the coal properties in the 'Single Coal Properties' window assuming that the default subbituminous coal adequately represents the PRB in this case. Be sure to re-select the 'Wall-Fired' furnace type in the 'Furnace Conditions' window to load the default LOI and furnace conditions for the different coal. Proceed to the

‘Calculate’ window. For the subbituminous, the predicted stack Hg emission rate is 2.9 lb/TBtu, which represents an overall removal of 63.3 % Hg.

The next series involves addition of $CaCl_2$ on the PRB coal to determine the levels of halogen injection required to capture similar levels of Hg as with the bituminous coal, determined above. For these cases, all selections are identical to the PRB case above, except that ‘Cl Addition’ is selected in the ‘Mercury Controls’ window under the ‘Standard Mercury Controls’ on the left of the screen or by checking the box under ‘Halogen’ in the right box. Either selection defines coal/in-furnace addition of Cl, which is suitable for this situation. Next cycle through the ‘Furnace Conditions’ window and make sure that the default properties for a subbituminous coal appear. The different levels of $CaCl_2$ addition are entered in the ‘Mercury Control Parameters’ window. The default values are an agent halogen content of 63.9 wt %, corresponding to $CaCl_2$, alongwith an agent coal loading of 300 ar ppmw. Execute the cases by selecting the ‘Calculate’ window after progressively altering the agent coal loading from 50 to 600 ppmv. These results are shown in Table 3.4, below.

Finally, examine the effect of Cl addition on a 50:50 PRB/bituminous coal blend. This test case is setup and executed in the same manner as for the PRB coal above, with three exceptions: (i) Select “<Blend>” from the ‘Single Coal Properties’ window; (ii) In the ‘Coal Blend Properties’ window, alter the coal-Cl for the bituminous coal to 0.054; and (iii) In the ‘Furnace Conditions’ window, select the ‘Wall-Fired’ furnace and change the LOI to 1 wt. %. Run parametric variations of $CaCl_2$ addition levels, as before. These results are shown in Table 3.4.

Table 3.4.Impact of $CaCl_2$ addition on a PRB and a 50:50 PRB:bituminous blend fired into an SCR+ESP+WFGD configuration.

Case	$CaCl_2$ ppmw on coal	Coal-Cl arppmv	Hg Removal %
Bituminous	0	0.054	83.9
PRB	0	0.010	63.3
	50		65.2
	200		70.8
	400		78.2
	600		85.5
50:50 PRB/Bit	0	0.032	73.8
	100		77.0
	300		83.4

Case 4, Discussion

The bituminous coal shows a high inherent Hg capture of 83.9 % because of its ample coal-Cl and the presence of an SCR in the gas cleaning system. For the PRB coal, the inherent Hg removal is only 63.3 %. This removal progressively increases when $CaCl_2$ is added to the PRB coal. To achieve a similar level of Hg removal, the PRB coal requires approximately 600 ppmw $CaCl_2$ addition. The target is much easier to meet with the 50:50 blend, because both the inherent fuel-Cl and LOI are greater. Note, however, that the effect of LOI is only marginal in this case because the SCR is the most effective Hg^0 oxidizer in the system. Consequently, adding 300 ppmw $CaCl_2$ to the blend provides sufficient Cl to obtain comparable Hg removals to the bituminous coal.

Case 4, Extensions

Repeat this study for ACI into a cleaning system with the SCR bypassed; i.e., into an ESP+WFGD. Use an ACI rate of 5 lb/MMacf for the PRB and PRB/bituminous blend. Adjust the $CaCl_2$ loading to achieve the Hg removal with the bituminous coal. Is $CaCl_2$ addition more effective in the SCR/ESP/FGD combination or in the ESP+WFGD combination with ACI? Repeat the entire series with $CaBr_2$ instead of $CaCl_2$. Why is Br addition so much more effective than Cl addition?