

## **Optimization as a Tool to Reconcile Performance Test Data**

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### **ABSTRACT**

In a power cycle performance test, measured results have uncertainties. A new method for reconciling these uncertainties is suggested. Critique and testing are required in order to validate or to reject this idea.

The idea is to “reconcile” the uncertainties in the test data using PEPSE®’s optimization tool. Thus optimization here is suggested for use in fitting the test data in the analysis process, rather than forcing an exact match, as is done in the “old” deterministic method. This is a non-traditional application of the optimization methodology. The application works by minimizing an objective function (a residual of weighted deviations between calculated and expected values of selected quantities). To accomplish this minimization, a set of test data points is chosen whose values are used/adjusted to obtain the minimization (maximization).

Example applications are included showing successes of the concept.

## INTRODUCTION

In a power cycle performance test, measured results have uncertainties. There are several sources of uncertainties. Among these are instrument error, calibration drift, hypothetical degradations in the process, and others. For analysis and interpretation purposes these uncertainties need to be reconciled. A new method is suggested to reconcile these measurement uncertainties. The result is a fit of the data.

An older deterministic method has existed and has been used for quite some time. PEPSE provides input options to use the test results directly, as-is. Generally when these options are used, there is some chosen unknown quantity in the system that is allowed to “float” in order to “close” the system analysis. In effect this floating quantity is the reconciliation. It absorbs all of the uncertainties of the measurement and the analysis. As a consequence, confidence in this quantity may be poor. For example, it is standard practice in analyzing performance tests of steam turbine cycles to “swing” the low-pressure (LP) turbine’s expansion line until the calculated power generation matches the measured power generation. Thereby the LP turbine’s efficiency is determined, sort of. This is done because measurements are not sufficient to determine the state point of wet steam that exists at the end of the LP turbine.

A new, alternative procedure is offered for consideration, using PEPSE’s optimization tool. The idea is to “reconcile” the test data uncertainties by fitting the test data in the analysis process, rather than forcing an exact match, as is done in the “old” method.

The application requires selection of an objective function to be minimized. The optimization tool permits the user to define an objective function that can be a single parameter in the model’s calculation or a weighted combination of parameters in the model. In the present suggested application, the objective function could be a composite of weighted deviations/residuals between PEPSE-calculated quantities and high confidence measured quantities, such as system power generation.

To complete the definition of the optimization's application, a set of "independent",  $x$ , variables would be chosen, that will be used/adjusted to obtain the minimization. In this application, these  $x$ 's are the variable names for the test data values that are uncertain. When the calculation is complete, in the general application, none of the values of the results of the calculation will match the measured quantities precisely. Instead, the analytical results, in the context of the heat balance model, are a "fit" of the data, but the fit may represent a superior result compared to the old, deterministic approach.

This idea is offered for critique and testing. At this stage its general applicability is unknown, and its worthiness relative to other approaches is unknown. Additional work and applications are required in order to answer this implied question. In particular, selection of a "good" objective function appears to be critical to obtaining a successful result.

Several example applications are used in this paper for demonstration purposes. Inasmuch as very limited "test data" are entered into a model that is otherwise theoretical, these are not realistic cases. Nevertheless, the examples are useful in providing understanding of the concept of application.

## **THE OPTIMIZATION TOOL**

In Version 65/GT4.0 and later, PEPSE includes a tool for optimization computations. This is a "special feature" that allows a modeler to choose any variable in a model for minimization or for maximization, the  $y$ , objective function. To accomplish this minimization, the modeler can select a set of " $x$ " variables in the model that PEPSE is requested to adjust. As an example, the  $y$  could be heat rate, and a single  $x$  might be condenser pressure for a steam turbine cycle model. The general application may include more than a single  $x$ , if desired.

A central aspect of the method of calculation of the optimum is the running of many cases by PEPSE, each case having a fixed set of values of the  $x$ 's, while recording the resulting  $y$  value. Before running a new case, PEPSE uses an algorithm for minimization to adjust the values of the

x's in a direction that is expected to reduce y. That is, the x values are "dithered", and the change of y is monitored.

The optimization procedure includes the option to place limits/constraints on each one of the x's to prevent unreasonable and non-physical values of x.

## HOW THE TOOL CAN APPLY TO TEST DATA

Within a tested system, one can choose a group of measured quantities that are desired to be matched as closely as possible by PEPSE's calculated results. A composite of these could form the y variable. For example, symbolically we could say:

$$y = a_1 * \text{abs}(y_{1m} - y_{1c}) + a_2 * \text{abs}(y_{2m} - y_{2c}) + \dots + a_n * \text{abs}(y_{nm} - y_{nc}) \quad (1)$$

that is the objective function, y is a linear combination of deviations/residuals of up to n different individual variables. If we could make y go to zero, we would then have an exact match between measured and calculated y's. In the Equation 1:

a<sub>1</sub> is a constant, weighting factor for the first y, and so forth for a<sub>n</sub>'s

y<sub>1m</sub> is the measured value of the first y, and so forth through y<sub>nm</sub>

y<sub>1c</sub> is the computed value of the first y, and so forth through y<sub>nc</sub>

The a<sub>n</sub>'s are constants whose values are chosen to give appropriate (equal?) numerical importance to each one of the y<sub>n</sub> terms.

We can use the optimization feature to attempt to minimize y in Equation 1. In actual application the input protocol for the optimization feature handles only a single y variable. However, a composite y, as in Equation 1, can be formed by using PEPSE operations to combine the y<sub>n</sub>'s of choice as shown in Equation 1. The final y would be saved in an operational variable, e.g. OPVB,102, and this variable would be declared to the optimizer as its y variable.

For input in a complex analysis task, each one of the measured values of  $y_n$  could be entered as operational variables also. Entering the values in operational variables has the desirable effect that the values are accessible for evaluation, as in Equation 1, but they would not be used directly in PEPSE's normal thermodynamic computations, except as we choose.

A simple example application can illustrate the idea. The target for matching could be the measured gross power generation (a single  $y$ ) for a modeled steam turbine system. The measured value could be input to PEPSE as the value for OPVB, 1. The  $y$  of Equation 1 could be computed by a user-defined operation, then

$$y = 1.0 * \text{abs}(\text{BKGROS},0 - \text{OPVB},1) = \text{OPVB},102 \quad (2)$$

This, OPVB, 102, would be specified to the optimization feature as the  $y$ , objective function name.

Continuing this simple example, we may be trying to determine an uncertain measured main steam flow rate, in order to match this measured generation (supposing that everything else in the system is "known"). In this case, the specification of the single  $x$  variable for the optimization feature would name WWVSC for the source/input component where main steam is introduced to the steam turbine cycle model.

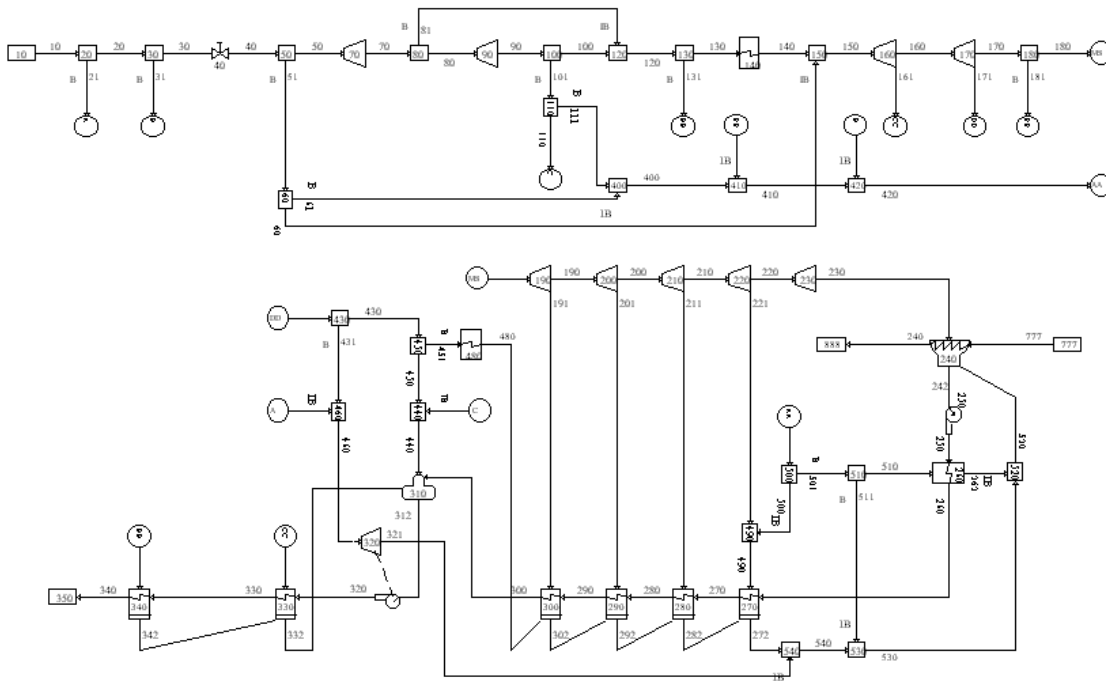
The experienced PEPSE modeler will realize that this simple example could be solved directly in PEPSE by use of a control. For the demonstration here, it is convenient to retain the simplicity to demonstrate the idea of application of the optimization feature to solve the problem. Once we understand the idea of application, it is a quick transition to consider applications to more complex/real circumstances.

The challenge in the general application is to assemble a meaningful and sufficient definition of  $y$ , along with an appropriate collection of  $x$ 's to attain a useful application and one that the optimization algorithm is capable of solving. This will not always be routine. There are

limitations to the number of x's that can be defined in an optimization application. There are also practical limitations to the ability of the algorithm to solve complex problems.

## FIRST APPLICATION

Consider a case based on an existing PEPSE model. For this discussion, we use the “fossil” model that is included with delivery of PEPSE software; the schematic here is Figure 1. In a test, two quantities have been measured, the power at 625 mW and the main steam flow at  $4.25 \times 10^6$  lbm/hr. It is assumed here that the model reliably represents the remaining details at the time of the test, that is the “true performance” of the system.



**Figure 1 Fossil Steam Turbine Cycle PEPSE Schematic**

For this application, the power generation will be regarded as “truth”, while the measured main steam flow value is uncertain. The task is to find a consistent value of main steam flow for the known generation. The optimization tool is used to reconcile these data.

Table 1 shows the input form for the optimization feature's use in the model.

**Table 1 Graphic Screen Showing Optimization Specification**

**Y Variable and X Variable**

**G Variable (Optional)**

**Y Objective Function Variable**

Description:

Variable Name:  Variable ID:   Minimize  Maximize

Convergence Criterion:  Number of cycles:

	X Variable Description	Variable Name	Variable ID	Start - First Value	Start - Second Value
1	MAIN STEAM FLOW	WWVSC	10	4100000.0	4400000.0
2			0	0.0	0.0
3			0	0.0	0.0

**Options**

Iterate to begin debug printing:  Maximum number of cases:

Case to begin debug printing:   Print standard results for each case

Cycle to begin debug printing:

Deletion status (enter DELETE to disable)

As seen in Table 1, the y function is OPVB,102, and the x is WWVSC,10. Observe also that two starting values are given for the flow rate. These are bracketing the expected final answer, but that is not a requirement. Also, the number of cycles is set to 3. This is “insurance” that a true minimum of the objective function has been found. In one cycle, the algorithm finds a minimum. In the next cycle, the search for minimum starts over again from a new set of starting points. Again a minimum is located. The third cycle starts with yet a third set of starting points. By this repetition, there is greater confidence that a true minimum has been found.

Table 2 shows the input forms for definition of OPVB,102 that is the objective function in the optimization feature.

**Table 2a Graphic Screen Showing Operation for Power Deviation**

**Minimum Data**

**Optional Data**

**OPERATION DEFINITION DATA (88NNN0)**

Description:

Result = f(first variable, second variable), where f() is the operation.

Operation:

	Name	ID	Optional multiplier
First variable	<input type="text" value="BKGROS"/>	<input type="text" value="0"/>	<input type="text" value="0.0"/>
Second variable	<input type="text" value="ONE"/>	<input type="text" value="0"/>	<input type="text" value="625.0"/>
Result variable	<input type="text" value="OPVB"/>	<input type="text" value="101"/>	<input type="text" value="0.0"/>

Required only for gas properties operations:

ID number of modeled stream carrying a fluid to be evaluated by gas property operations:

The simplicity of this analysis application has motivated skipping the use of OPVB,1 (Equation 2 above) for the measured value of power. Instead, the value is hard-wired into the operation as a multiplier of 625.



**Table 2b Graphic Screen Showing Operation for Absolute Value of Power Deviation**

**Minimum Data**

**Optional Data**

**OPERATION DEFINITION DATA (88NNN0)**

Description: **ABSOLUTE VALUE OF DEVIATION**

Result = f(first variable, second variable), where f() is the operation.

Operation: **ABS**

	Name	ID	Optional multiplier
First variable	ONE	0	0.0
Second variable	OPVB	101	0.0
Result variable	OPVB	102	0.0

Required only for gas properties operations:

ID number of modeled stream carrying a fluid to be evaluated by gas property operations:

**RESULTS FOR FIRST APPLICATION**

With the operations and optimization definition shown in the previous section, PEPSE was run to convergence to find the reconciled main steam flow rate. The value was found to be 4.226e6 lbm/hr. Table 3 shows the output from the optimization calculation.

**Table 3 Output Table Showing Results of Optimization Calculations for First Application**

V-GT5C (97 STEAM TABLES) OF 11 APR 00 DATE 04/12/01. PAGE 27  
 FINAL OPTIMIZATION CASE, CYCLE 3, CONVERGED. 39TH CASE, THIS CYCLE  
 \*\* SAVE CASE \*\*

OPTIMIZATION CALCULATION RESULTS  
 C..FOSRXYL(SET 11)-RECONCILE MAIN STEAM FLOW, OPTIMIZING MW DEVIATION

VALUE	DESCRIPTION	UNITS
	Y OBJECTIVE FUNCTION OPTIMIZED:	
9.406E-06	OPVB ( 102), ABSOLUTE VALUE, MW DEVIATION	OPVB
	X INDEPENDENT VARIABLES:	
4.226E+06	WVSC ( 10), MAIN STEAM FLOW	BM/HR

As presented by the table, OPVB,102 is equal to 9.4e-6. This is the absolute value of the deviation between the measured and calculated power in mW. The optimization process went through three “cycles” with a total of 125 cases being run in order to reach this solution. The run time on a Pentium III-500 PC computer was 47 seconds.

**SECOND APPLICATION**

The second application builds on the first one. In this instance, it is desired to minimize the combined deviations of measured power and measured flow rate from the calculated values. Furthermore, it is to be assumed that both quantities have an uncertainty of +, 2%.

The setup of this analysis task is similar to the First Application, but there are some additional details. Now the objective function is a composite, as depicted in Equation 1 above. Furthermore, there are constraints to be placed on the variables.

The specification of the optimization feature is shown in Table 4. Note that there are three displays shown here in order to include the constraints. Table 4a shows the basic optimization setup. It is virtually the same as Table 2a. Now the objective function is OPVB,105, instead of OPVB,102, and a value of convergence criterion has been set to override the built-in criterion. Table 4b shows the constraints on main steam flow, and Table 4c shows the constraints on generation. Each of these defines a band of +/- 2%. Notice that, because power generation is not (and, as a computed variable, not an input variable, cannot be) one of the x variables in the optimization, the constraints on power, shown in Table 4c, are “general variable” constraints. As a consequence, the constraint on power will be informative only. The constraint on main steam flow will restrict the final answer for x, flow rate, to be within the bounds specified for the x constraint.

**Table 4a Main Inputs for Optimization for Second Application**

**Y Variable and X Variable**

**Y Objective Function Variable**

Description: **WEIGHTED MW AND FLOW DEVIATION**

Variable Name: **OPVB** Variable ID: **105**  Minimize  Maximize

Convergence Criterion: **0.0001** Number of cycles: **3**

	X Variable Description	Variable Name	Variable ID	Start - First Value	Start - Second Value
1	MAIN STEAM FLOW	WWVSC	10	4100000.0	4300000.0
2			0	0.0	0.0
3			0	0.0	0.0

**Options**

Iterate to begin debug printing: **0** Maximum number of cases: **150**

Case to begin debug printing: **0**  Print standard results for each case

Cycle to begin debug printing: **0**

Deletion status (enter DELETE to disable)

OK Cancel Steam Tables...

Table 4b Optimization Form Showing Main Steam Flow Constraints

FDSRXYL.MDL, Optimization: Set: 12

Y Variable and X Variable      G Variable (Optional)

Y Objective Function Variable

Description: **WEIGHTED MW AND FLOW DEVIATION**

Variable Name: **OPVB**      Variable ID: **105**       Minimize     Maximize

Convergence Criterion: **0.0001**      Number of cycles: **3**

	Variable ID	Start - First Value	Start - Second Value	Constraint Minimum	Constraint Maximum	Disable
1	10	4100000.0	4300000.0	4165000.0	4335000.0	<input type="checkbox"/>
2	0	0.0	0.0	0.0	0.0	<input type="checkbox"/>
3	0	0.0	0.0	0.0	0.0	<input type="checkbox"/>

Options

Iterate to begin debug printing: **0**      Maximum number of cases: **150**

Case to begin debug printing: **0**       Print standard results for each case

Cycle to begin debug printing: **0**

Deletion status (enter DELETE to disable)

OK      Cancel      Steam Tables...

**Table 4c Optimization Form Showing Power Constraints**

	G Variable Description	Variable Name	Variable ID	Constraint Minimum	Constraint Maximum	Dis
1	GENERATOR POWER	BKGROS	0	612.5	637.5	
2			0	0.0	0.0	
3			0	0.0	0.0	
4			0	0.0	0.0	
5			0	0.0	0.0	
6			0	0.0	0.0	
7			0	0.0	0.0	
8			0	0.0	0.0	
9			0	0.0	0.0	
10			0	0.0	0.0	

As seen in Table 4a, the objective function,  $y$ , for optimization is now OPVB,105. Operations, as shown in Table 5, are used to construct this quantity as a linear, weighted combination of the power deviation and the main steam flow deviation. The operations of Table 2 above still apply to the formation of the power generation deviation and are not repeated here. However, Table 5 shows the forms for the three operations that are used to calculate main steam flow deviation and then to combine it with the power generation deviation, in variable OPVB,105. In creating the objective function, the main steam flow deviation is “normalized”/weighted so that the numerical values are not more important than the power deviation. This normalization occurs by multiplying the main steam deviation by the factor  $1.47e-7$ . This was developed from the measured power and flow values as

$$\text{Factor} = 625/4.25e6/1000$$

No claim is made that this is the best or the only weighting factor that should be used. Experimentation could be useful.

**Table 5a Form for Operation to Compute Main Steam Flow Deviation**

FOSRXYL.MDL, Operation : 103, Set : 12

**Minimum Data**      **Optional Data**

**OPERATION DEFINITION DATA (88NNN0)**

Description:

Result = f(first variable, second variable), where f() is the operation.

Operation:

	Name	ID	Optional multiplier
First variable	<input type="text" value="WWVSC"/>	<input type="text" value="10"/>	<input type="text" value="0.0"/>
Second variable	<input type="text" value="ONE"/>	<input type="text" value="0"/>	<input type="text" value="4250000.0"/>
Result variable	<input type="text" value="OPVB"/>	<input type="text" value="103"/>	<input type="text" value="0.0"/>

Required only for gas properties operations:

ID number of modeled stream carrying a fluid to be evaluated by gas property operations:

Table 5b Form for Operation to Compute Absolute MS Deviation

FOSRXYL.MDL, Operation : 104, Set : 12

Minimum Data      Optional Data

**OPERATION DEFINITION DATA (88NNN0)**

Description: ABSOLUTE VALUE OF MS FLOW DEVIATION

Result = f(first variable, second variable), where f() is the operation.

Operation: ABS      Select operation ...

	Name	ID	Optional multiplier
First variable	ONE	0	0.0
Second variable	OPVB	103	0.0
Result variable	OPVB	104	1.47e-7

Required only for gas properties operations:

ID number of modeled stream carrying a fluid to be evaluated by gas property operations: 0

OK      Cancel      Steam Tables...

**Table 5c Form to Calculate Composite, Weighted MW and MS Deviations**

FOSRXYL.MDL, Operation : 105, Set : 12

**Minimum Data** | Optional Data

**OPERATION DEFINITION DATA (88NNN0)**

Description:

Result = f(first variable, second variable), where f() is the operation.

Operation:

	Name	ID	Optional multiplier
First variable	<input type="text" value="OPVB"/>	<input type="text" value="102"/>	<input type="text" value="0.0"/>
Second variable	<input type="text" value="OPVB"/>	<input type="text" value="104"/>	<input type="text" value="0.0"/>
Result variable	<input type="text" value="OPVB"/>	<input type="text" value="105"/>	<input type="text" value="0.0"/>

Required only for gas properties operations:

ID number of modeled stream carrying a fluid to be evaluated by gas property operations:

**RESULTS FOR SECOND APPLICATION**

With the operations and optimization definition shown in the previous section, PEPSE was run to convergence to find the reconciled main steam flow rate. The value was found to be 4.226e6 lbm/hr. Table 6 shows the output from the optimization calculation.

As seen in Table 6, the results are substantially the same as those in the first application above. Examination of further details in the output of the two applications shows that the main steam flow rates are identical. In addition, the specified constraints were not violated for either the main steam flow rate or for the power generation.



**Table 6 Output Table Showing Results of Optimization Calculations for Second Application**

V-GT5C (97 STEAM TABLES) OF 11 APR 00 DATE 04/12/01. PAGE 27  
 FINAL OPTIMIZATION CASE, CYCLE 3, CONVERGED. 47TH CASE, THIS CYCLE  
 \*\* SAVE CASE \*\*

OPTIMIZATION CALCULATION RESULTS  
 C..FOSRXYL(SET 12)-RECONCILE MS FLOW BY OPTIMIZING MW AND MS FLOW DEV

VALUE	DESCRIPTION	UNITS
	Y OBJECTIVE FUNCTION OPTIMIZED:	
3.546E-03	OPVB ( 105), WEIGHTED MW AND FLOW DEVIATION	OPVB
	X INDEPENDENT VARIABLES:	
4.226E+06	WWVSC ( 10), MAIN STEAM FLOW	LBM/HR

**THIRD APPLICATION**

In the previous applications, the optimization feature has worked when there were only two variables involved, power generation and main steam flow rate, with main steam flow rate being the x variable. This third application examines the possibility of success when additional variables are involved.

In this application, additional “test data” are considered. To those already considered, we add the measured hot reheat temperature, 997 F, which is regarded as uncertain, and the temperature at the second extraction from the LP turbine, 498.5 F, which is regarded as “truth”. These new measured values can be used much as in the applications above. For sake of brevity, the forms for specifications of optimization feature and operations are not shown here.

The objective function was defined as a linear combination of the absolute values of the deviations of predicted and measured values of power generation and LP turbine extraction temperature. Now there are two x variables. These are the main steam flow rate and the hot reheat temperature.

In the interest of keeping it simple, this application is treated most like the first application above. Unlike the second application, no accounting is made of constraints that might be dictated by specified uncertainties of the test data.

### **RESULTS FOR THE THIRD APPLICATION**

A run to obtain the solution of the optimization task produced the result shown in Table 7. The main steam flow rate is  $4.229\text{e}6$  lbm/hr, and the hot reheat temperature is 998.5 F. Further examination of the output file reveals that the measured power generation of 625 mW and the LP extraction temperature of 448.5 F, variables that compose the objective function, were matched nearly identically. This is also observable in the table below where the magnitude of the objective function is seen to be  $1.7\text{e-}4$ .

**Table 7 Output Table Showing Computed Results of Optimization for Third Application**

V-GT5C (97 STEAM TABLES) OF 11 APR 00 DATE 04/12/01. PAGE 27  
 FINAL OPTIMIZATION CASE, CYCLE 3, CONVERGED. 62TH CASE, THIS CYCLE  
 \*\* SAVE CASE \*\*

OPTIMIZATION CALCULATION RESULTS  
 C..FOSRXYL(SET 13)-RECONCILE MS FL AND HRH T BY OPT MW AND LP EXT

VALUE	DESCRIPTION	UNITS
	Y OBJECTIVE FUNCTION OPTIMIZED:	
1.749E-04	OPVB ( 105), WGTD MW PLUS LP EXT T DEVIATION	OPVB
	X INDEPENDENT VARIABLES:	
4.229E+06	WWVSC ( 10), MAIN STEAM FLOW	LBM/HR
9.985E+02	TTTORH( 140), HOT RH TEMPERATURE	DEG F

For the record, the mW and LP extraction temperature weightings in the objective function were equal at 1.0.

This run required one minute and fourteen seconds on the PC computer.

**WHAT DID NOT WORK**

In the second application, the optimization series did not converge using the default convergence criterion. To help it converge, the convergence criterion was increased from 1.e-5 to 1.e-4. The default value, which is fractional, is just too tight when the value of the objective function is tending toward zero.

The first attempt to run the third application did not include the “known” LP extraction temperature. The objective function was simply the deviation between measured and calculated power generation. As defined, the method would not reach a converged solution. Deeper consideration tells us that there are an infinite combination of main steam flow rates and hot reheat temperatures that will give us 625 mW of power. Looked at another way, we can say that there were two unknowns, the flow rate and the HRH temperature, while there was only a single

“known” (“equation”). So, it was necessary to introduce a second “known”, this being the “trusted” value of LP extraction temperature.

## **ALTERNATIVE TO THE USE OF OPTIMIZATION**

PEPSE’s control feature is an effective tool for analyzing the three applications discussed above. The one aspect that is not covered by controls is the use of constraints to represent uncertainties. Additional runs were made using controls, and the results duplicated those that have been presented here. For each application, only a single case was required; thus making the solutions by controls are faster than those by optimization.

It is likely that the optimization tool would be more useful than controls for reconciliations involving more variables.

## **CONCLUSIONS**

This paper has shown that the optimization feature can be used to “fit” performance test data by adjusting values of uncertain data. As mentioned above, the examples in this paper were also solved more directly and quickly by using PEPSE controls. It remains to be investigated whether more complex and useful applications (that would be unsolvable by controls) are workable by the optimization tool.

Defining a meaningful objective function is one of the challenges facing effective use of the optimization tool. Including enough trusted values for matching, to provide sufficiency for the solution, may be an issue. Our training in mathematics tells us that, for each unknown, there needs to be a known, an equation, to be able to solve. Also, optimization calculations, by their intense computational nature, can be unpredictable and may frequently terminate without convergence. More experience is needed in order to decide whether this can be a useful application. The appendix presents an academic example of an optimization assignment. This exercise is included for demonstration purposes. It has no relationship to heat balances for power generation systems. It does demonstrate the need for care in selecting objective functions.

Because of the structure of running PEPSE, the optimization method to reconcile test data would not work in the context of PEPSE's widely-used Special Option 6. There is a conflict because the optimization procedure creates its own series of stacked cases that would interfere with the required stacked-cases structure of SO6.

## **BIBLIOGRAPHY**

Minner, G, et al, "PEPSE Volume 1 User Input Description", SCIENTECH, Inc., Idaho Falls, Idaho, 2000.

## **APPENDIX - CAUTION**

The optimization tool is a powerful method for finding the minimum/maximum of the declared objective function. One must always be cautious about the results from analysis. It is a good idea to be skeptical and to study the results. One way to do this is to check the sensitivity of the objective function to the x values by running a few separate trial cases while varying the x variables and observing the value of the objective function. If minimization was expected, the value of the objective function should always increase when moving away from the optimum "point".

One should be cautious of the possibility of having found a "local minimum", rather than the "global minimum" that is being sought. Doing a systematic spot check at points over the domain of physically realistic x's can improve confidence that the point found really is the optimum.

It is also a good idea to be thoughtful and careful about the choice of the objective function in seeking an optimum point. If you choose the "wrong" objective function, you may get the "wrong" optimum. The risks increase when the objective function is a composite of more than a single term, as it was in the second and third applications above.

To demonstrate this point, consider an optimization problem that is simple and easily understood, that can be posed to PEPSE's optimization tool, and that can be solved independently by calculus. This is the case of a cylindrical can made of sheet metal. The goal of the optimization is to find the combination of diameter and length of the can that minimizes the amount of metal that is to be used in making a container of a given volume. The amount of metal is minimized by minimizing the surface area of the can. This is a classic problem from calculus. We can write the equations for the volume and the area and rearrange and take the derivative of the area with respect to diameter and set this derivative to zero. We can also pose this as an optimization assignment to PEPSE assisted by the use of operations to set up the computations.

Below, the symbols are:

- V = volume
- VG = given volume
- VC = calculated volume
- A = total surface area
- D = diameter of the ends
- L = length of the cylindrical surface portion
- OF = objective function
- C1 = weighting factor
- C2 = weighting factor

The volume of the can is

$$V = \left[ \pi * D^2 / 4 \right] * L \tag{1}$$

$$A = 2 * \left[ \pi * D^2 / 4 \right] + \pi * D * L \tag{2}$$

For manipulations for calculus evaluation, we can solve (1) for L and substitute the result into (2)

$$L = 4 * V / (\pi * D^2) \tag{3}$$

$$A = [\pi * D^2 / 2] + 4 * V/D \tag{4}$$

If we now take the derivative of A, in equation (4) with respect to D and set this equal to zero and solve, we get the diameter that minimizes the area:

$$D = \text{cube root } (4 * V/\pi) \tag{5}$$

For a unity volume, the diameter is

$$D = 1.0839$$

$$L = 1.0839$$

For analysis by PEPSE, we can make a simple submodel with a source and a sink, that serve only to have a model for PEPSE. “The real problem” is solved, then, by encoding our volume, length, and area calculations as operational variables and operations. That is, V, D, L, and A are declared as operational variables, OPVB,101, OPVB,102, OPVB,4, and OPVB,7, respectively. Equations (2), (3), and (4) are programmed using operations. This has been done, and the optimization tool has been activated, with A (OPVB,7) as the y objective function and D (OPVB,102) as the x variable. Starting and ending values of D were 0.5 and 2.0, respectively. Constraints on D were 0.1 and 10. The results from running this case was

$$D = 1.082$$

$$L = 1.088$$

This differs from the exact answer because of the tolerance allowed by the convergence criterion.

Now, consider a different way of solving this problem that has some resemblance to the applications discussed for the fossil model above. We will recast the analysis with the volume calculated based on diameter and length of the can, and we will choose D and L as two different

x's in the optimization. That is, Equation (1) will be used instead of Equation (3). In order to assure attaining the desired volume, we will form a composite objective function that includes the surface area and the deviation of the volume from the desired volume.

$$OF = C1 * A + C2 * \text{abs}(VG - VC) \quad (6)$$

Running PEPSE to minimize this objective function would appear to give us the solution that we desire. Certainly if  $VC = VG$ , that part is minimized. So, we try  $C1$  and  $C2$  equal 1.0. The result of this analysis produced the following result:

$$D = 0.1$$

$$L = 0.1$$

Which provided an area and volume of nearly zero. Thus  $OF$  was nearly 1.0. This is not the answer we were expecting! What happened? If we look at the answer that we “know” and put it in (6), we find that  $OF$  would be about 5.5, because the volume difference is zero, and the surface area is all that remains. So, we conclude that we picked a bad objective function. Reasoning tells us that the volume deviations's weighting is not big enough. So, we could try  $C2$  equal 100, while  $C1$  stays at 1.0. We get a solution, but not the right solution. So we try  $C2$  equal 5 and  $C1$  equal to 10. When we do this, the answer comes out to be close and closer to the expected answer.

Our conclusion from this experimentation is that caution is important when developing an objective function that is a composite of variables, such as the deviations from expected values. The recommendations at the beginning of this appendix become important for these types of cases.