**Module 3**

**Industrial Sector Level Management: Pollutant Trading using multicriteria optimization and decision making under uncertainty**

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**Problem statement:**

Total Maximum Daily Load (TMDL) of 32.8 kilograms/year for mercury has been established by the USEPA for five contiguous segments of the Savannah River in the state of Georgia, US, leading to the applicable water quality standard (WQS) of 2.8 ng/l (parts per trillion) in the watershed. 29 major industries (point sources) need to comply with this water quality standard. The U.S. Environmental Protection Agency (EPA) defines point source pollution as “any single identifiable source of pollution from which pollutants are discharged, such as a pipe, ditch, ship or factory smokestack”. Three different mercury control technologies, namely, activated carbon adsorption, coagulation and filtration, and ion exchange, are available for installation. Each of these technologies has a different cost and mercury reduction capability. Since the cost of compliance for the individual industries is typically high, it has been proposed to explore mercury trading as an option.

Trading is mostly practiced in a decentralized manner for other pollutants. However, a decentralized trading mechanism has following limitations:

1. Point sources will typically overachieve the reduction targets due to technology specifications when trading is not possible. This reduces the overall mercury discharge more than that mandated by the regulation. However, when trading is allowed, the overall reduction will be equal to that mandated by the regulation. The actual magnitude of this difference cannot be estimated with decentralized trading.
2. The emissions, even though satisfying the regulatory requirements, will lead to some health impacts on the human population. The government/regulatory agency need to know the impact of allowing trading on the overall health care costs. This cannot be accomplished in a decentralized manner.

Therefore, it is desired to develop an integrated optimization based framework to administer mercury trading in the considered watershed.

The specific goal is to formulate an optimization model to determine the optimal trading policy among the 29 point sources and to select the most appropriate control technologies for individual point sources, with the objective of reducing the overall compliance cost for all the point sources together. It is also desired to extend the basic optimization model to consider nonlinearity in control technology cost functions and uncertainty in parameter values. We also want to consider the impact of trading on overall health care cost of the population consuming water in the watershed and formulate an optimization model that balances the compliance cost and the health care cost.

**Specific activities for optimization model formulation**

1. Identify and list the model parameters for which data are given
2. Identify the decision variables in the model
3. Formulate the model constraints
4. Formulate the economic objective function (cost minimization)
5. Calculation of the health care cost due to exposure to mercury
6. Program the model in a software tool (GAMS)
7. Exercise: Solve the model and analyse the results

**Solution**

We will first formulate a generic optimization model and then apply it to the specific case of the Savannah River basin.

The TMDL (Total Maximum Daily Load) regulation has already been developed by the state in consultation with USEPA. This translates into a specific load allocation for each point source. Consider a set of point sources (PS*i*), *i* = 1,…,*N*, disposing pollutant containing waste water to a common water body or a watershed. The various point source specific parameters are:

*Di* = Discharge quantity of polluted water from PS*i* [volume/year]

*ci* = Current pollutant concentration in discharge water from PS*i* [mass/volume]

*redi* = Desired pollutant quantity reduction in discharge of PS*i* [mass/year]

*Pi* = Treatment cost incurred by PS*i* to reduce pollution when trading is not possible (obtained from module 2)

Let *j* = 1,…,*M* be the set of waste reduction technologies available to the point sources. The technology specific parameters are:

*fj*(*ϕj, Di*) = Cost function for total plant cost for technology *j* [$]

*qj* = Pollution reduction possible from the implementation of technology *j* [mass/volume]

where, *ϕj* is the set of design parameters of technology *j*.

Pollutant trading requires the regulatory agency to fix two parameters that govern the trading. These are trading ratio and transaction fee. Trading ratio decides how many units of pollutant reduction a source must purchase to receive credit for one unit of load reduction. Ideally, trading ratio should be 1 since the pollutant everywhere is treated equally. However, there are often uncertainties about the actual reductions achieved at different point sources. Therefore the trading ratio *r* is usually set higher than 1 to account for data uncertainty and provide a buffer. Consequently, the PS accepting additional discharge reduction responsibility has to reduce the pollutant by an amount equal to the actual quantity traded times the trading ratio. Transaction costs are the expenses for trading participants that occur only as a result of trading. This could include documentation and approval expenses and so on. We will make the following assumptions:

* Trading is possible between all point sources.
* The trading ratio *r* and transaction fee *F* (in $/mass) is the same for all possible trades

The decision variables are:

* *bij*: Binary variable representing point source-technology correlation. The variable is 1 when PS *i* installs technology *j*, and 0 otherwise.
* *tik* (mass/year): Amount of pollutant traded by PS *i* with PS *k*, i.e. PS *i* pays PS *k* to take care of its own pollution.

All the parameters are on annual basis.

Once the model parameters and decision variables have been identified, we then need to formulate the model constraints and the objective function. Constraints in an optimization model are conditions such as mass balance and energy balance that must be satisfied by the solution. Objective function provides the target for the optimization problem solution. The constraints and objective function are modelled here:

1. **Constraint 1:** No point source can perform a trade with itself and hence we need to introduce the following constraint:

This constraint will force the variable corresponding to the amount traded between the same point source to be zero. Note that the constraint is repeated for all *N* point sources.

1. **Constraint 2:** It needs to be ensured that the prescribed regulatory limits are satisfied with or without trading. Since trading is options, it is possible that some industries will perform a trade while others will not. We, therefore, need a constraint that ensures that the desired pollutant quantity reduction for a point source (*redi*) is met considering both these possibilities. The constraint is modelled as follows:

Here, the left hand side is the total reduction target for point source *i*. the first term on the right hand side is the amount of reduction achieved by installing a waste reduction technology *j* at point source *i*. When the model is solved, the binary decision variable *bij* will govern which reduction amount is selected for point source *i*. Note that all *bij* may be zero. The second term on the right hand side indicated the quantity of pollutant that is purchased by the point source from another point source *k*. This is the quantity that point source *k* is reducing on behalf of point source *i*. Therefore, it is considered as contributing towards the reduction target of point source *i*. It is also possible that point source *i* is reducing discharge on behalf of another point source *k* and trading that amount. The last term on the right hand side captures such a possibility after adjustment for the trading ratio. Note that the last term has a negative since that is the amount traded by point source *i* on behalf of industry *k*. Therefore, that amount should not be considered as contributing towards achieving the reduction target of point source *i*. Please note that the indices on variable *t* are reversed for the last two terms on the right hand side, and that the constraint is included for all point sources. It also needs to be noted that all the terms may not have a non-zero value in the final solution.

1. **Constraint 3:** Since pollutant trading is optional, a point source will participate in trading only if it leads to an overall economic gain for that point source. Thus, for a point source *i*, the total cost incurred after participating in trading must not be higher than *Pi,* the treatment cost incurred by PS*i* to reduce pollution when trading is not possible (obtained from module 2). This is modelled by the following constraint:

Here, the first term on the right hand side is the cost of installing the waste reduction technology, and the second term on the right hand side is the cost of performing trading. Note that the trading cost needs to be paid for both inward and outward trades. The inequality sign ensures that this total cost incurred while trading cannot be more than the cost incurred without trading.

1. **Objective function:** The objective of pollutant trading, as stated earlier, is to reduce the overall compliance cost for the set of point sources. Therefore, the objective function for this optimization problem is:

The objective function is the sum of the waste reduction technologies installed across all the point sources in the considered region. Although each point source will also spend or gain from practicing trading, expense for one point source in a watershed is earning for one or more point source in the same watershed. As a result, for the complete watershed, trading does not contribute to the cost objective. Hence, the objective function does not include any term depended on the transaction fee *F*.

A simple cost function is linear with respect to the amount of waste being treated. For such cases, the cost function can be written as:

Here, represents the treatment cost per unit volume for technology *j* ($/volume)*.*

1. **Health care cost calculation:** The discharge of mercury to the watershed is still to humans, particularly because of its bioaccumulative nature. Even though the total discharge is below the TMDL regulation (with or without trading), population consuming water will still be exposed to mercury. Therefore, it is expected that some health care cost would be incurred. It is important consider this health care cost while comparing different solutions of the proposed optimization model. This is especially important since different geographical regions (such as states within a country) have different laws leading to differing effective health care costs (essentially different value of human life). Since trading can have implications on the locations of the industry, the understanding of this trade-off can contribute in sound policy making. We will, therefore, develop the equation to calculate the health care cost due to the mercury discharge in the watershed.

The bioaccumulative nature of mercury and its slow dynamics make the long term effects of mercury exposure important. Hence, it is essential to account for such effects while quantifying the health care costs. Majority of mercury accumulates in the food chain as methyl mercury. Therefore, quantification of the health care costs based on methyl mercury concentration is most appropriate. IRIS (Integrated Risk Information System) database reports methyl mercury reference dose for chronic oral exposure (RfD), which is the highest dose of methyl mercury without any harmful effects. However, since the TMDL for the Savannah River is developed on the discharge of total mercury to the watershed, not just methyl mercury, the model needs a quantifying measure based on total mercury. IRIS database does not report the RfD value for mercury (elemental). Therefore, we will quantify the health care costs through LC50 (Lethal Concentration 50%) value for mercury. LC50 is defined as the concentration of a toxic substance (mercury) at which 50% of the population exposed to it dies within a certain time. LC50 value of a substance is often used to quantify its harmful exposure effects.

The health care cost is a function of the final overall mercury discharge. This discharge value is used to calculate average mercury consumption by humans. This value is then compared with the mercury consumption rate at which 50% human population will die (calculated using the LC50 value). The comparison gives an approximate estimate of human mortality rate due to discharge of mercury in the watershed.

The presence of mercury in water is dangerous to humans primarily through fish consumption. During the development of TMDL for Savannah watershed, it has been established that a WQS of 2.8 ng/liter leads to safe mercury concentration in fishes (). We will assume a linear relationship between WQS and average mercury concentration in fishes. Therefore, knowing the actual WQS after compliance () gives the average fish tissue mercury concentration after compliance. The calculation of can be done as follows. Let represent the final reduction achieved by each point source, which may be more than the mandated target of . is calculated as:

We can then calculate as follows:

Then, knowing the average fish consumption per person per day in the watershed (), the total mercury intake by an individual is computed. Thus, mercury intake per person per day in grams is given as:

This mercury intake rate is to be compared with the rate resulting in 50% mortality. Since the LC50 value for humans is not available, we will assume that the value for the fish being consumed by humans in the watershed is close to the value for humans. The most commonly consumed fish in Savannah watershed is largemouth bass. It is assumed that chronic exposure to mercury is through consumption of contaminated water by humans. If is the average water consumption per person per day, then the consumption rate leading to 50% mortality can be computed. The 50% lethal consumption rate per person per day in grams is given as:

Let *P* be the population in the watershed affected by mercury pollution, and be the health care compensation per mortality. Then the total health care cost for the watershed is given as:

The health care cost can be used to compare different optimization solutions, in which case the cost is calculated post-optimization. It is also possible to modify the optimization problems presented before by including the health care cost as a part of the objective function.

1. **Additional constraint:** It should be noted that the model developed here can also be used to solve the case where trading is not possible or not allowed in the watershed. In order to enable that, the following constraint can be added to the formulation:

This constraint forces the variable corresponding to the amount of mercury traded between all possible point source combinations to zero. This indirectly implies that trading is not possible in the watershed. Therefore, the solution of such a problem will give the costs and technology selection options for the case without trading (Module 2).

One can also put a constraint on the number of mercury control technologies an industry can select. In a realistic scenario, an industry will prefer to select a single more technology rather than two or more different technologies. This is because the operating constraints and the technical knowhow for two different technologies might be vastly different. The model can therefore be modified to include such as constraint as follows:

This constraint ensures that only one of the binary variables is non-zero for each industry. Note that multiple installations of the same technology, such as two ion exchange processes connected in series, are not considered. The model can be extended to model multiple such installations by considering another set of integer variables. This is left as an exercise for students to solve.

**Programming of the model in GAMS**

The module provides a separate tutorial for programming an optimization model in GAMS (General Algebraic Modeling System). Screenshots for the programming of mercury trading problem in GAMS are provided (Figures 1-4). The GAMS editor along with the educational version of the license can be freely downloaded from the GAMS website ([www.gams.com](http://www.gams.com)). The free educational version can solve problems up to a maximum of 300 constraints and 300 variables. For larger problems, a solver specific to the problem being solved needs to be purchased. Students can also use the NEOS server (<http://www.neos-server.org/neos/>) hosted by the Wisconsin Institutes for Discovery at the University of Wisconsin in Madison and provides access to several solvers free of charge. The user has to formulate and code the model in GAMS on the local machine. The problem can then be submitted to the NEOS Server (please see the NEOS guide on the website), where it is solved and the results are reported.

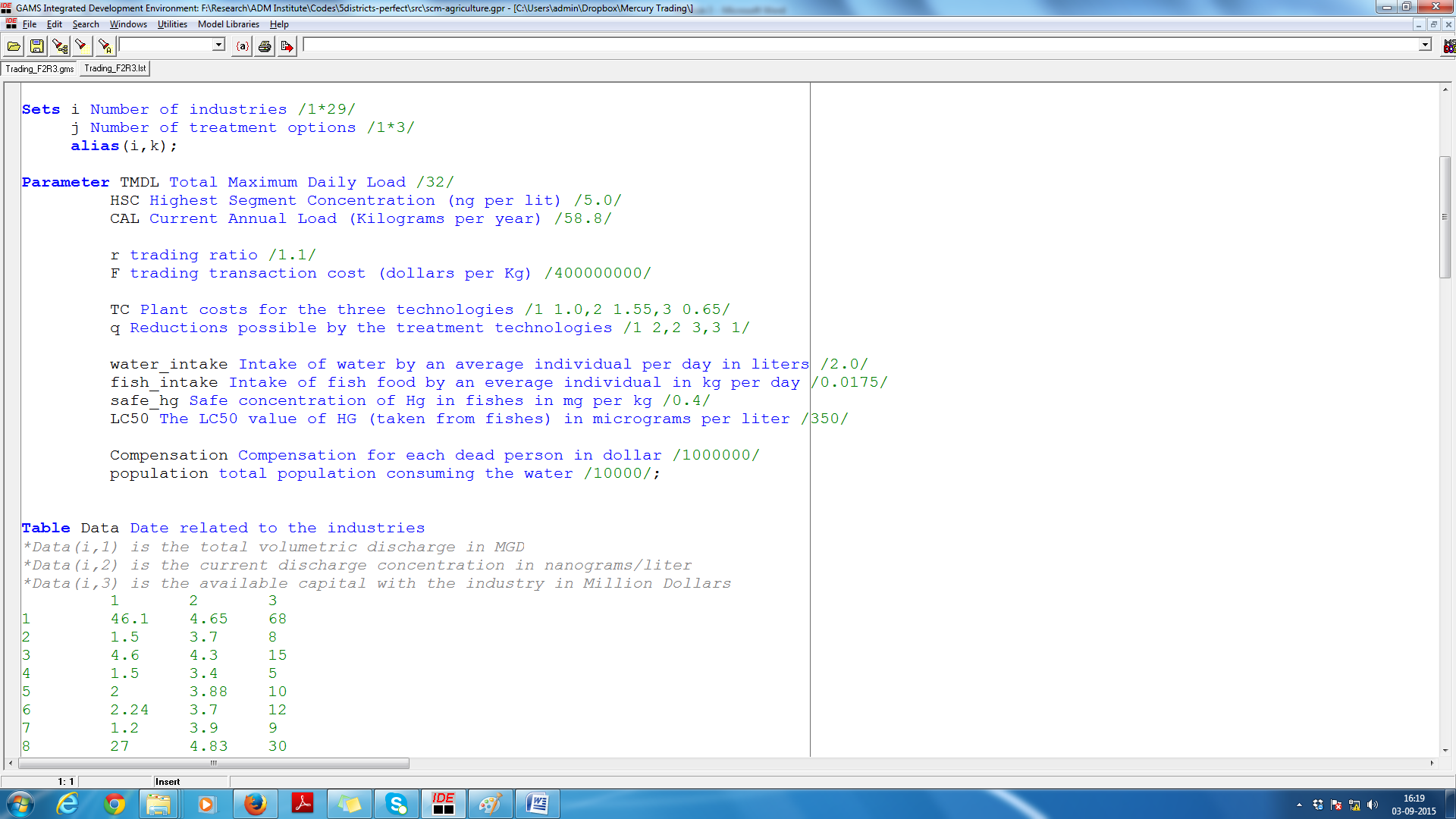


Figure 1: Declaration of sets and parameter values for model formulation

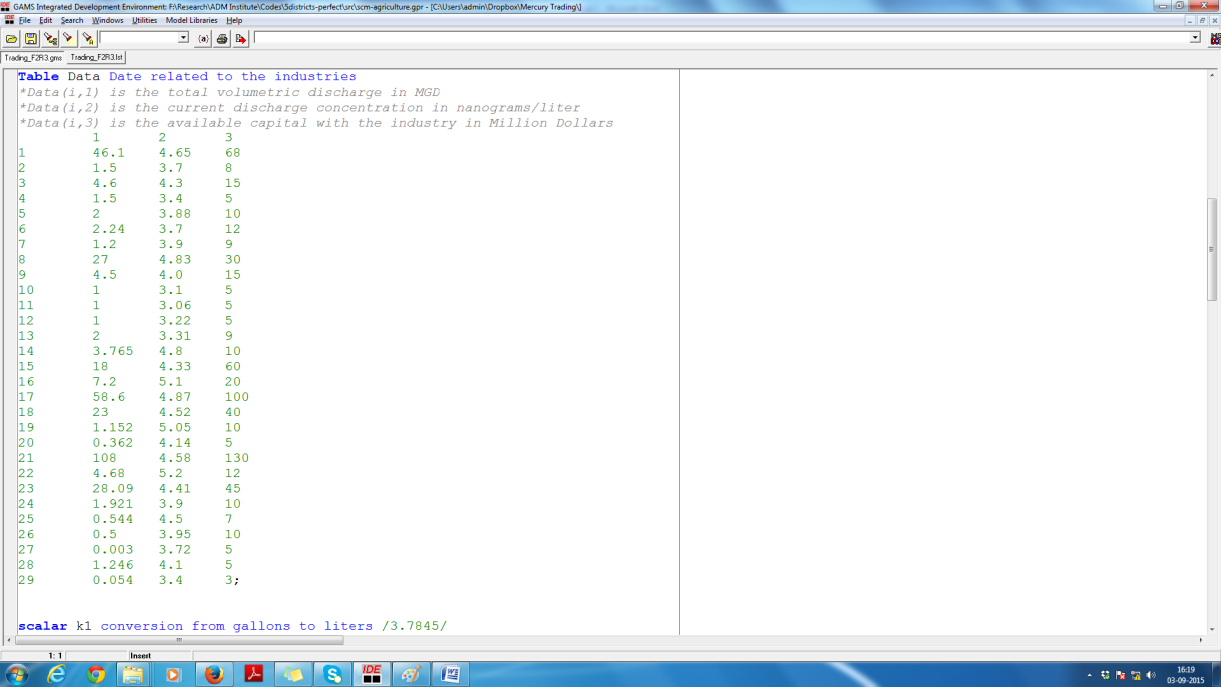


Figure 2: Declaration of data table for 29 point source industries

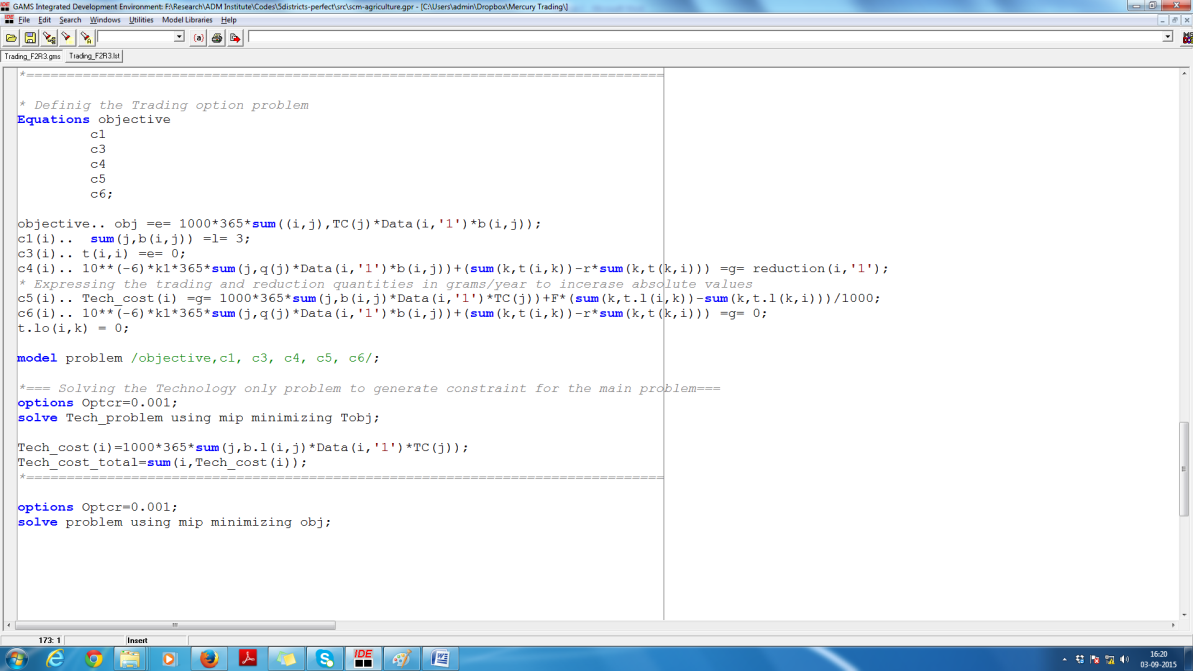


Figure 3: Declaration of equations, model and solve statement

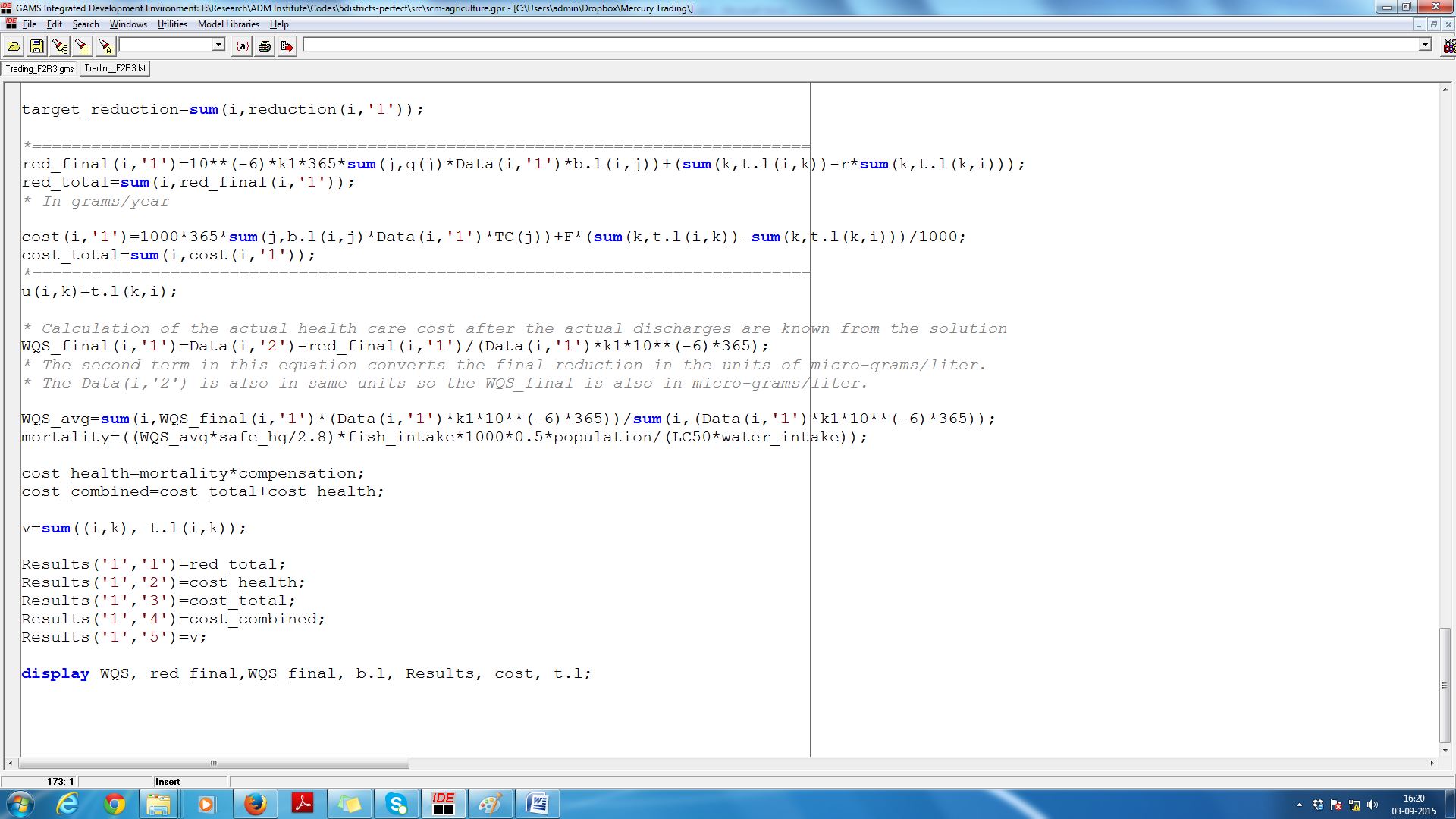


Figure 4: Post optimization calculation of health care cost for the model simulation result

**Exercise: Model solution and analysis of results**

The model that we have formulated and programmed in GAMS is to be used to solve the given case study. In particular, the important questions of interest that need to be answered are:

1. What is the percentage reduction in the overall compliance cost for the 29 point sources due to the possibility of trading in the watershed?
2. What is the total quantity of mercury traded in the watershed?
3. What are the preferences for the selection of technology among the three options? How does this change with trading is allowed as against when trading is not allowed?
4. What is the impact of trading on total health care cost for the watershed?
5. How do these results change if the value of the TMDL is changed? The model can be solved for values of 26 kg/y to 36 kg/y (base case value is 32 kg/y).

**Modified Problem statement: Health care cost objective**

The consideration of health care costs in the comparison of the trading problem solution is an important factor while studying the impact of pollutant trading on the watershed. In the previous exercise, we have seen that permitting trading will change the overall health care cost for the watershed as compared to when trading is not permitted. Therefore, in order to conduct a thorough assessment, we can include the health care cost as part of the objective function of minimization. The optimization model can then be solved again to see if there is any change in the solution.

**Specific activities for modeling problem statement:**

1. Modify the objective function to include health care costs
2. Solve the problem with the modified objective and compare the solutions
3. Perform sensitivity analysis with respect to the weight of the health care cost in the objective function

**Solution:**

Let be the total health care cost for the watershed as determined by the equation given in the previous exercise. Then the modification of the objective function will be as follows:

Here, is the weightage given to the health care cost in the objective function. The purpose of this weighting coefficient is twofold:

1. The weighting coefficient allows the modeller to solve the model with different levels of importance given to the health care costs in the objective function. The default value of is 1. However, as the value increased, the importance of health care cost increases.
2. The proposed model is a multi-objective o/multi-criteria optimization model where the objective function consists of two very different types of components. In this case, these are compliance costs and health care costs. For such problems, the two components of the objective function can often different by orders of magnitude and hence one term may dominate another. In such cases, the weighting coefficient enables the modeller to ensure that the orders of magnitude are same.

The remaining constraints remain the same.

**Exercise: Model solution and analysis of results**

In this exercise, the important questions of interest that need to be answered are:

1. What is the solution when health care cost is considered as part of the objective?
2. How does the solution change when we solve the model for different values of ?

**Modified Problem statement: Nonlinearity and uncertainty**

The earlier formulation assumed a linear cost function of the mercury control technologies, i.e., the cost of technology implementation scales linearly with the volume of waste being treated. Simplified linear models, while being computationally advantageous, may lead to gross qualitative and quantitative errors in optimal results. Nonlinear models, on the other hand, provide more accurate representation, but result in computationally challenging problems. Inclusion of uncertainty is also governed by a trade-off between accuracy and computational simplicity. Correct characterization and quantification of uncertainty is equally important for reliable results. Consequently, for the proposed decision making framework to be successful, an extensive analysis of these modeling related issues is essential. We will, therefore, modify the model to incorporate nonlinearity and uncertainty in the problem formulation.

**Specific activities for modeling problem statement:**

1. Modify the optimization model formulation to include nonlinear cost functions of the mercury control technologies
2. Solve the optimization model with nonlinear cost functions
3. Identify important parameters in the nonlinear cost functions that might be uncertain (not known deterministically).
4. Modify the optimization model to include uncertainties in nonlinear cost functions, leading to the formulation of a stochastic optimization problem
5. Modify the problem formulation into a two stage stochastic programming problem
6. Modify the GAMS code to incorporate the formulation change
7. Solve the two stage stochastic programming problem in GAMS to generate results

**Nonlinear problem formulation:**

The formulation of the optimization problem with nonlinear cost functions is simple. Instead of a linear cost model, the cost of a particular mercury treatment technology is calculated using a nonlinear model. The detailed nonlinear cost models are provided in the appendix B. These need to be added to the problem formulation and become the constraints of the optimization model.

**Exercise: Nonlinear problem solution**

In this exercise, the important questions of interest that need to be answered are:

1. What is the impact of considering the detailed nonlinear cost models on the results? These impacts should be with respect to the compliance cost, health care cost, technology selection, amount of material traded, and the simulation time.
2. How do the results for the nonlinear cost function change for different TMDL values? The model can be solved for values of 26 kg/y to 36 kg/y (base case value is 32 kg/y). How is this trend as compared to the one for the linear cost models?

**Identification of uncertain parameters:**

There are multiple parameters in each of the nonlinear cost models that can potentially be uncertain. However, we will focus on a limited set of parameters that are important in the model and are more likely to be uncertain in nature. The parameters selected for uncertainty analysis are:

**Coagulation and filtration:**

* Cost per membrane
* Electricity rate
* Cost of sodium hypochlorite
* Membrane life

**Granular activated carbon process:**

* Coefficients to compute the capital and operating costs

**Ion exchange process:**

* Resin price
* Two coefficients representing the slope and intercept to compute the tank total cost

Once the uncertain parameters have been identified, we need to decide the natural of uncertainty and the degree of variability. The nature of uncertainty implies the probability distribution of the uncertain parameter. Several possible distributions include uniform, normal, log-normal, and triangular and so on. The selection of a particular distribution depends on the information available about the possible values of the parameter. If no specific values are available, of if values available do not indicated any specific distribution, normal or uniform distribution are often considered. Once the nature of the probability distribution is known, we need to decide the properties of the distribution such as mean and standard deviation. These values will fix the degree of variability, and the values should ideally depend on real data.

**Stochastic problem formulation:**

The optimization model presented in the previous section assumes that all data is deterministically known. However, there are various possible sources of uncertainty in this framework. At the TMDL development step, the discharge from individual point sources, and fate and transportation of mercury is variable. These will affect the final bioaccumulation results, and hence the regulations and discharge allocations. Moreover, data related to many mercury treatment technologies can be uncertain. This can either be due to uncertain performance characteristics of the technology (e.g., conversion efficiency, catalyst life), or due to relatively scarce data about a new treatment technology. This leads to considerable uncertainties about the technology performance and cost. Under these circumstances, one has to work with the available data to arrive at optimal decisions. In optimization terminology, this is known as stochastic optimization (stochastic programming). We will, therefore, extend the nonlinear deterministic model by considering uncertainties in nonlinear technology cost functions formulation and solution methodology.

Let *uj* represent the uncertain parameters for control technology *j*. Therefore, the cost function is given as . For a stochastic optimization problem, the objective function is then converted into an expectation function. Therefore, the modified stochastic optimization problem is given as:

Subject to:

Here, *E* in the objective function is the expectation operator over the set of uncertain parameters *uj.* All other notations have been previously defined as part of the linear or nonlinear formulation. Since the cost functions are nonlinear, this problem is a stochastic mixed integer nonlinear programming problem.

For solving the model, the model is converted into a two stage stochastic programming problem. The basics of this two stage decomposition have been covered in the introductory section. Accordingly, the two stage problem is formulated as follows:

**Master (stage-1) problem:**

Subject to

Where, represents the first stage objective function. The first three constraints of the problem are same as those for the linear or nonlinear deterministic problem formulated previously. Please note that in the first stage problem, we approximate the nonlinear cost functions using a linear model. However, that is done indirectly, where the linear models put a bound on the cost. The fourth constraint puts a lower bound on the linear approximation of the nonlinear cost models using the previously used linear cost functions. The last constraint represents the optimality cut that is generated during each iteration of the sub-problem (described below). This optimality cut includes the first stage decision variables of and , which are collectively represented as in the equation above.

The first stage decisions are passed on to the second stage (sub-problem) where the recourse function is computed using nonlinear models. Here, the uncertain variables are sampled *Nsamp* times, and the second stage sub-problem is solved for each sample to calculate the expected value of the nonlinear recourse function. The second stage problem is thus given as:

**Sub (stage-2) problem:**

Subject to

Here, represents the exact cost computed using the nonlinear cost models for a particular sample *n* of the uncertain parameter set *uj*. The solution of the second stage problem results in a possible generation of an optimality cut, which is included in the subsequent master problem solution through the computation of and matrices.

**Programming of the stochastic problem in GAMS:**

There is an important modification required to the GAMS code in order to solve the proposed two stage stochastic programming problem. The decomposed stochastic programming problem needs to be solved iteratively. The solution of the stage 1 master problem approaches the real optimal solution with each iteration. The master and sub-problems mentioned here, therefore, need to be a part of a “for” loop that is executed for a large number of iterations. The code to write the “for” loop can be found in the provided GAMS codes.

Sampling can be done by using the existing sampling methods available in GAMS. GAMS allows you to specify the probability distribution along with the distribution specific parameters. For example, “uniform(1,2)” will lead to samples that are uniformly distributed between 1 and 2, the lower and upper bound, respectively.

**Exercise: Stochastic problem solution**

In this exercise, the important questions of interest that need to be answered are:

1. What is the impact of considering the uncertainty in cost models on the results? These impacts should be with respect to the compliance cost, health care cost, technology selection, amount of material traded, and the simulation time.
2. How do the results for the stochastic cost models change for different TMDL values? The model can be solved for values of 26 kg/y to 36 kg/y (base case value is 32 kg/y). How is this trend as compared to the one for the linear cost models?

**References for further reading**

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