# A mathematical optimization technique for managing selective catalytic reduction for coal-fired power plants \*

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Abstract Selective catalytic reduction (SCR) is an emissions control technique that primarily reduces harmful emissions of oxides of nitrogen ( $NO_x$ ). To maintain SCR performance, catalyst layers maybe added, removed, or replaced to improve  $NO_x$  reduction efficiency. To make these changes, power plants must be temporarily shut down, and SCR maintenance during scheduled power plant outages can be very expensive. Consequently, developing a fleet-wide SCR management plans that are both efficient at reducing  $NO_x$  and limiting operating costs would be extremely desirable. We propose an SCR management framework that finds an optimal SCR management plan that minimizes  $NO_x$  emissions using integer programming. The SCR management tool consists of two main modules—the SCR schedule generation module and the SCR optimization module. Furthermore, the SCR management framework addresses decision making from the fleet-wide perspective as well as a single plant as opposed to only a single plant, which is currently commercially available. We demonstrate the effectiveness of the tool and provide a tradeoff between  $NO_x$  reduction and operating cost using Pareto optimal efficient frontiers.

**Keywords** Mathematical optimization  $\cdot$  Integer linear programming  $\cdot$  Energy management  $\cdot$  Selective catalytic reduction

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#### 1 Introduction

Coal is considered as one of the most important energy sources in the U.S. It is accountable for roughly half of the electricity we use and one fourth of our total energy [19]. However, it is also the single biggest industrial air polluter in the U.S [3]. One of the major emissions generated from coal combustion is oxides of nitrogen ( $NO_x$ ): in a year a typical coal plant will generate around 10,200 tons of NO<sub>x</sub> [3]. NO<sub>x</sub> leads to the formation of ozone, which inflames the lungs, burning through lung tissue and making people more susceptible to respiratory illness [10]. NO<sub>x</sub> also leads to fine particle formation and acid precipitation. In addition, nitrogen dioxide causes health impacts in and of itself, and thus is one of the six regulated criteria pollutants. The US Environmental Protection Agency (EPA) has steadily tightened regulations for allowable amounts of pollutants that can be discharged into the atmosphere [10]. For fossil fueled power plants, regulations are now in place for the amounts of sulfur dioxide (SO<sub>2</sub>), carbon monoxide (CO), volatile organic compounds (VOCs), particulate matter (PM), and NO<sub>x</sub> that can be released into the atmosphere. Equipment and operating modifications can reduce NO<sub>x</sub> emissions. Technologies such as low NO<sub>x</sub> burners, staged combustion, gas recirculation and low excess air firing can all assist with NO<sub>x</sub> removal. However, to meet upcoming EPA mandates, more aggressive reduction techniques, such as Selective Catalytic Reduction (SCR), will need to be used [10].

SCR is an emissions control technique with the primary purpose of converting  $NO_x$  in exhaust gases into harmless nitrogen gas and water. The SCR process consists of injecting ammonia (NH<sub>3</sub>) into boiler flue gas and passing the flue gas through a catalyst bed where the  $NO_x$  and  $NH_3$  react to form nitrogen and water vapor [3]. As the SCR reduces  $NO_x$ , its performance deteriorates. To maintain the performance, SCR catalyst layers maybe added, removed, or replaced to improve  $NO_x$  reduction efficiency. However, to make these changes, the power plant must be temporarily shut down, so SCR maintenance occurs during scheduled power plant outages, which are expensive. Consequently, developing a fleet-wide SCR management plans that are both efficient at reducing  $NO_x$  and limiting operating costs would be extremely desirable.

In this paper, we describe an SCR management framework that provides an optimal SCR plan during scheduled outages for all plants in the fleet, given an existing plan of scheduled outages. Section 2 discusses how electricity is generated in coalfired power plants, and Section 3 describes the current literature on SCR management. In Section 4, we discuss the SCR management tool, including a description of SCR reactor potential and  $NO_x$  reduction in Section 4.1, the SCR schedule generation module in Section 4.2, and the SCR optimization module in Section 4.3. We discuss the effectiveness of the tool with computational experiments in section 5. Finally, Section 6 describes conclusions and future directions.

# 2 Electricity Generation Process

The basic process of a coal-fired power plant is to convert the chemical energy in coal into thermal energy or heat, thermal energy into mechanical energy of a turbine, and mechanical energy into electrical energy. Figure 1 displays an overview of a coal-fired power plant. Coal from the mine is pulverized and delivered by a conveyor belt

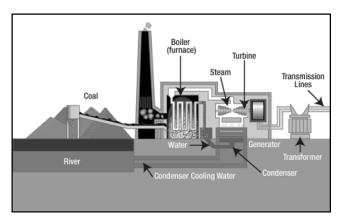


Fig. 1 An overview of a coal-fired power plant [2]

to the boiler where a mixture of coal and air ignites. Intense heat from the burning coal converts a large amount of water in the boiler into steam, which spins the turbine to generate electricity. In addition, there are numerous sub-processes associated with the boiler (not shown in Figure 1).

Burning coal produces harmful emissions (e.g.,  $NO_x$ , PM, and  $SO_2$ ), which are vented from the process (not directly from the boiler).  $NO_x$  are formed when molecular nitrogen and oxygen naturally occurring in the air combine at the high temperatures present in the boiler (thermal  $NO_x$ ), and when nitrogen in the coal is oxidized during the combustion process (fuel  $NO_x$ ). Many of these harmful emissions can be decreased using a variety of emissions control technologies. For example,  $NO_x$  emissions at the stack can be significantly reduced through SCR technology. In Figure 1, the SCR would be implemented between the boiler and the stack. In the SCR,  $NO_x$  emissions travel through a series of catalytic layers to react with ammonia ( $NH_3$ ). This reaction can convert  $NO_x$  and  $NH_3$  into harmless byproducts, mainly nitrogen and water. We refer to the  $NO_x$  that comes from the boiler as *inlet NO\_x*, and the  $NH_3$  injected into the SCR as  $NH_3$  *injection*. Not all of the inlet  $NO_x$  and  $NH_3$  injection reacts in the SCR, and the remaining  $NO_x$  and  $NH_3$  are referred to as *outlet NO\_x* and  $NH_3$  *slip*, respectively.

The amount of outlet  $NO_x$  and  $NH_3$  slip depend upon the potential reactivity of the catalyst in the SCR, which degrades over time. As the SCR degrades,  $NH_3$  injection is ramped up to maintain reasonable levels of outlet  $NO_x$ , but this increases  $NH_3$  slip as well. Since high levels of  $NH_3$  exposure is hazardous to humans, it is necessary to maintain low levels of  $NH_3$  slip. In addition, Increased  $NH_3$  injection

in turn affects the long-term performance of the SCR:  $NH_3$  slip can form particles which could potentially corrode downstream equipment and can cause plugging in the SCR, which can be expensive to maintain. Overuse of  $NH_3$  injection is also expensive. Therefore, optimal SCR management involves adding and/or removing catalyst layers during scheduled outages, so as to maintain high levels of SCR potential reactivity and thereby control  $NO_x$  emissions,  $NH_3$  slip, and operating costs across multiple plants. Specifically, the problem is to find an optimal SCR plan that minimizes  $NO_x$  emissions given a scheduled outage plan for each plant where during these outages catalyst layers maybe added or removed and replaced to improve  $NO_x$  reduction efficiency.

#### 3 Literature Review

In this section, we provide an overview of literature related to SCR management and existing applications that can be found in industry.

Staudt and Engelmeyer [21] stated that the objective of optimized catalyst consumption is to minimize the catalyst costs and optimize the operation of the facility simultaneously to achieve the lowest cost to produce power. This objective leads to many trade-offs such as catalyst consumption, the frequency and duration of outages,  $NH_3$  slip,  $NO_x$  reduction, and baseline  $NO_x$ . They also define catalyst activity as the ability to facilitate the  $NO_x$  reducing reactions. Over time, the impurities in the gas stream will deposit on the catalyst and block exhaust gas from reaching active sites within catalyst.

Based on Muzio, Quartucy, and Cichanowicz [13] and Pritchard et al. [17], there are three major factors that affect the catalyst deactivation. The first factor is sintering of the catalyst due to high temperatures. The second factor is due to alkaline metals, earth metal masking, and/or arsenic oxide. The last factor is catalyst plugging.

From Staudt and Engelmeyer's study [21], "Most SCR reactors are designed with up to four available levels of catalyst. When the system is new, with fresh catalyst, at least one level is typically empty as shown in Figure 2." When the SCR performance drops to an unacceptable level, which occurs around 2 years, a new catalyst level is added to the spare layer. Later, when SCR reactor potential drops again, an old catalyst level that generated the lowest activity is replaced with new catalyst. Thus, this will increase total catalyst activity.

According to Cichanowicz and Muzio [5], there are three options to maintain SCR performance. The first option is to install a new catalyst into a spare layer or replace the old layer with new catalyst. The second option is to install regenerated catalyst. This option has lower cost than the first option, but SCR performance will be lower when using regenerated catalyst than when using new catalyst. The last option is in-situ cleaning or regeneration. Cleaning is when a catalyst is taken out and clean thoroughly with chemical while regeneration is when catalyst is restored to a like new condition. This option can be done in a shorter period of time such as 2 to 3 days compared with other options, which require 2 to 3 weeks. Although, it can be done in a shorter period of time, the reactor potential will not be restored as with the other two options.

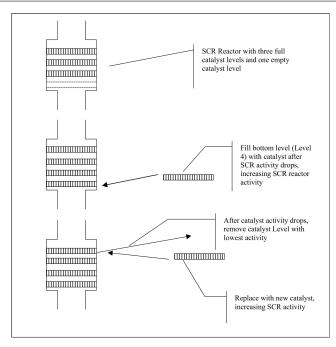


Fig. 2 Normal add and replace sequence [21]

Cichanowicz, Smith and Muzio [6] estimated the capital cost of SCR is \$125 per kW depending on the level of NO<sub>x</sub> reduction, type of catalyst, and complexity of the retrofit. Due to capital cost of catalyst replacement, the maintenance outage schedule, and the SCR performance, Cichanowicz, Smith, Muzio and Marchetti [7] provided five options as follows. The first option is to replace catalyst as planned. The second option is to delay catalyst exchange and increase NH<sub>3</sub> injection. The next option is to delay catalyst exchange and maintain NH<sub>3</sub> injection. The fourth option is to accelerate an outage for early replacement. The last option is to perform on-line cleaning. All of the above have pros and cons that cause the catalyst to be challenging to manage.

In terms of an alternative cost efficient method to SCR, Rubin, Salmento and Frey [20] discussed an effective emissions control for coal-fired power plants using integrated environmental control (IEC) concepts involving combined SO<sub>2</sub>/NO<sub>x</sub> removal processes in combination with pre-combustion and combustion control methods.

Pritchard and DiFrancesco [16] described SCR catalyst management with goals of NO<sub>x</sub> reduction, Hg oxidation, SO<sub>3</sub> emissions, and operation flexibility by physical inspection of the plants, collection of data and tests to predict the future performance. Jia Mi [12] optimized NO<sub>x</sub> emissions by using Computational Fluid Dynamics (CFD) for SCR coal-fired stream power plants to improve the chemical process of the system. Another way to improve the effectiveness of the chemical process is by using the NH<sub>3</sub> injection grid (AIG), which is essentially an optimization of the chemical process of NH<sub>3</sub> injection by adjusting the AIG [18].

Chen and Frey [4] optimized  $NO_x$  and operating costs of the SCR by process design using stochastic optimization and programming. They described methods for optimization of process technologies by considering the distinction between variability and uncertainty. These methods are developed and applied to case studies of  $NO_x$  control for integrated gasification combined cycle systems. Another related method described by Rubin, Diwekar and Frey [8] also optimized the process design using deterministic and stochastic optimization.

Grabitech [11] provided a NO<sub>x</sub> optimization software, multisimplex which is based on three different theories: evolutionary operation, simplex algorithms and fuzzy set theory. The basic idea in evolutionary operation is to replace the static operation of a process by a continuous systematic scheme of slight perturbations in the control variables. The effect of these perturbations is evaluated and the process is shifted in the direction of improvement similar to the Simplex algorithm. The fuzzy set theory allows several goals to be handled at the same time. Multisimplex calculates new settings for the next trial on the journey towards the optimum. Another widely used catalyst management tool is called CatReact [9] which was developed as part of an EPRI-sponsored collaboration between FERCo and JEC Inc. In contrast, our SCR management framework addresses decision making from the fleet-wide perspective as well as a single plant as opposed to only a single plant, which is currently commercially available.

# 4 SCR Management Framework

In this section, we describe an SCR management tool that optimizes  $NO_x$  reduction in a fleet of plants using SCR. The inputs to the tool include three text files—a plant file that includes information on the power plants, an outage file that includes information on the currently scheduled outages, and a parameter file that includes the fleet-wide information. These outages span over a predetermined time horizon that is usually about five years. The output is an optimal outage file in the same format as the inputted outage file with outages that span the same time horizon. An overview of the architecture of the tool is shown in Figure 3.

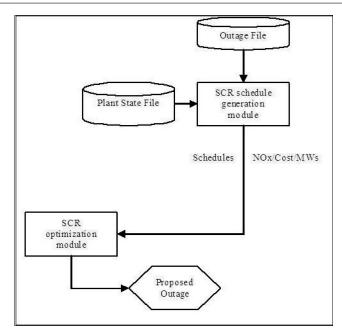


Fig. 3 An overview of SCR management tool architecture

The inputs to the tool can be categorized into four main categories, which are plant information, layer information, outage information, and global information. The summary of the input data information is shown in Table 1. Plant information includes

Table 1 Summary of input data information

Plant	Layer	Outage	Global
Information	Information	Information	Information
Plant number Number of installed SCR layers Power generation plan NH <sub>3</sub> slip Minimum NO <sub>x</sub> reduction Maximum operating costs Inlet NO <sub>x</sub>	Degradation rate Blockage rate Volume Surface area Catalyst activity Flue gas flow rate Dates of last activity	Start date End date Plant number Action Layer number	Fleet-wide constraints Fleet-wide parameters High budget Low budget Number of Pareto points

characteristics of each plant, which can be different from plant to plant. The number of installed SCR layers is the number of layers installed at the beginning of the time horizon. This number is used to determine the SCR reactor potential as well as the change and add sequences as shown in Fig. 2. The position of these layers which are filled from bottom to top also affect the degradation rates and blockage rates as shown in Fig. 1, where the closer the catalyst layers to the boiler, the higher degradation and blockage rates. Power generation plan is used as a constraint where each plant would need to meet the minimum fleet-wide power generation plan as specified by the users.

NH<sub>3</sub> slip values are inputted in two levels; the level in which is the assigned plant is currently using and the maximum level allowed by the plant. These two levels are then used to generate schedules, which will be described in Section 4.2. Minimum NO<sub>x</sub> reduction is a constraint where each plant has to meet this required minimum. Maximum operating costs is the budget allowed per plant, which consist mainly of catalyst, labor, reagent, fan power, and electricity costs. These costs values are determined by plant, layer, outage, and users specified information. Inlet NO<sub>x</sub>, generally measured in pounds per hour, is the amount of NO<sub>x</sub> entering the SCR, which is used to find the amount of outlet NO<sub>x</sub> leaving the SCR by taking into the consideration of each filled layer information. Layer information includes specific characteristics of each layer, which can be different for each layer as well as plants. There are typically four available layer slots per plant where two slots are typically filled at the beginning of the time horizon. Degradation rate is typically given in guaranteed usage hours by the catalyst manufacturer. The number of actual hours can vary for each layer depending upon its operating conditions. The blockage rate is an exponential rate in which layers are blocked by ash and is calculated by the users or recommended by the manufacturer. Volume, Surface area, and catalyst activity are general characteristics of catalyst layers that determine the reactor potential. The flue gas flow rate is inversely proportional to the reactor potential so the higher the flow rate, the more frequent layers need to be changed. The dates of the last activity of each layer will determine how long the layer has been in the system. As a general rule, where all the layers slot are filled, the layer that has been in the system the longest will be changed first. If there is a tie, generally the layer closest to the boiler is the one that will be changed. These layer characteristics also depend upon the position slots and the distance away from the boiler. These will directly impact the SCR reactor potential, where the higher the reactor potential, the more NO<sub>x</sub> will be reduced. Outage information includes what is planned to be done for all outages in the time horizon. This information includes the start and end dates and the associate plant for each scheduled outage. Layer actions include catalyst additions or changes where the layers being added or changed can be new, regenerated, or cleaned. A new layer is a brand new layer that has not been used before, a regenerated layer is a used layer that has been restored very close to new layer conditions, and finally a cleaned layer is also a used layer that has been taken out and cleaned thoroughly with catalyst. These three types of layers have different operating costs and NO<sub>x</sub> reduction efficiency implications with the efficiency of the a new layer being greater than than of a regenerated layer, and that of a regenerated layer being greater than that of a cleaned layer. These outage information are used to generate time-lines which will be described in Section 4.2. After the time-lines are generated the SCR optimization module, which will be described in Section 4.3, will then select an optimal schedule for each plant during time time horizon. Global information includes all fleet-wide constraints and parameters that are associated with the whole fleet. These include minimum power generation, minimum NO<sub>x</sub> reduction, maximum operating costs, and the time horizon. High budget, low budget, and the number of Pareto points are used to determine the Pareto optimal efficient frontiers that will be discussed in Section 5.2.

The tool consists of two main modules, namely the SCR schedule generation module and the SCR optimization module. The SCR schedule generation module

enumerates a set of possible outage schedules, while the SCR optimization module selects an optimal set of these schedules. The SCR management tool was developed using Microsoft Visual C++ version 6.0.

## 4.1 SCR Reactor Potential and NO<sub>x</sub> Reduction

In this section, we describe equations for  $NO_x$  reduction and reactor potential (RP) that are used in the study. The policy that we have employed uses fixed levels of NH<sub>3</sub> slip based upon what the plants are currently operating. The NH<sub>3</sub> slip is fixed at two levels which are 2 part per million (ppm) and 4 ppm. For each generated schedule, which will be discussed in greater details in section 4.2, NO<sub>x</sub> reduction and RP will be calculated based upon the fixed NH<sub>3</sub> slip levels throughout the schedule at both 2 ppm and 4 ppm. This would yield two values of both NO<sub>x</sub> reduction and RP for each schedule. Using 4ppm of NH<sub>3</sub> increases NO<sub>x</sub> reduction and RP but also results in higher costs due to using more reagent. Consequently, there exists a tradeoff. If the objective is to minimize cost, then obviously the schedule that uses 2 ppm of NH<sub>3</sub> slip is more attractive. In contrast, if the objective is to maximize  $NO_x$  reduction, the optimization will likely choose the 4 ppm schedule. In some cases however, for a schedule that uses 2 ppm of NH<sub>3</sub> slip, NO<sub>x</sub> reduction might not exceed a required minimum specified by the user, which is typically 70%. In this case, the schedule which uses 2 ppm of NH<sub>3</sub> level would be removed, while the 4 ppm level would be selected as a potential candidate by the optimizer. The RP, a measure of the overall potential of the reactor to reduce  $NO_x$  for a given catalyst layer at time t, can be calculated as follows.

$$RP_{\text{layer}}(t) = \frac{K_0 e^{\frac{-t}{T}}}{A_{\nu}},\tag{1}$$

where  $K_0$  is the initial catalyst activity value  $(\frac{m}{hr})$ , T is the degradation rate of the catalyst (hr), and  $A_v$  is the area velocity  $(\frac{m}{hr})$ . In addition, the RP for a given unit at time t can be calculated as follows.

$$RP_{\text{unit}}(t) = \sum_{\text{layer} \in \text{unit}} RP(t).$$
 (2)

The percentage of  $NO_x$  reduction is an increasing function of  $NH_3$  and RP(t) and is given by

$$DNOX_{\%}(t) = f(RP_{\text{unit}}(t), NH_3slip(t)), \tag{3}$$

where  $NH_3slip(t)$  is the NH<sub>3</sub> slip at time t. As mentioned previously, we assumed that  $NH_3slip(t)$  is set at either 2 ppm or 4 ppm for all values of t. The formula for f is based upon the manufacturer of the catalyst, and the one used is this research is considered proprietary by the sponsor of the research. To find an anticipated daily NO<sub>x</sub> reduction and average RP for a schedule s, which will be discussed in section 4.2, we integrate over the time horizon as follows:

$$\overline{DNOX}_{s} = \int_{t}^{\overline{t}} \frac{InletNO_{x} \times DNOX_{\%}(t)}{\overline{t} - \underline{t}} dt, \tag{4}$$

$$\overline{RP}_s = \int_{t}^{\overline{t}} \frac{RP_s(t)}{\overline{t} - \underline{t}} dt, \tag{5}$$

where  $\underline{t}$  is the start of the time horizon,  $\overline{t}$  is the end of time horizon, and  $InletNO_x$  is the amount of inlet  $NO_x$  into the SCR. Observe that between two outages, average RP is given by

$$RP_{\text{unit}}(t) = \sum_{\text{layer} \in \text{unit}} \frac{T_{\text{layer}}(RP(\underline{t}) - RP(\overline{t}))}{\overline{t} - \underline{t}}.$$
 (6)

Consequently, average RP for a schedule can be derived by taking a weighted of average (6) between the outages. However, calculating average  $NO_x$  reduction requires numerical integration.

### 4.2 SCR Schedule Generation

The primary purpose of the SCR schedule generation module is to enumerate a set of possible outage schedules where each generated schedule includes the following characteristics:

- 1. One power plant to which the schedule pertains.
- 2. A set of outages from the inputted outage file that maintain the following qualities:
  - The first outage in the schedule is the same as the first outage of the currently scheduled outage of the power plant.
  - The last outage in the schedule is the last outage of one of the plants in the currently scheduled outages.
  - One SCR catalyst layer from the power plant will be either added or changed in each outage.
  - All consecutive outages in the schedule will be within a predetermined window of days apart, usually around 270 to 450 days.
- 3. The maximum level of NH<sub>3</sub> slip.
- 4. An anticipated average daily reactor potential (RP) of the schedule.
- 5. An anticipated average daily NO<sub>x</sub> reduction of the schedule.
- 6. An anticipated operating costs of the schedule.
- 7. An anticipated power generation of the schedule.

The first step in SCR schedule generation is to read in a set of original schedules. Each original schedule includes an original timeline and a set of parameters, like the amount of NH<sub>3</sub> slip. Each original timeline represents a sequence of outages assigned to the same plant. Each outage includes a starting time, an ending time, an originally assigned plant, and a catalyst layer decision. The potential catalyst layer decisions are: add a new layer, change the oldest layer, regenerate the oldest layer, or clean the oldest layer. The second step in SCR schedule generation is to enumerate a set of new timelines, using the two functions Generate Timelines and Find Timelines described as Algorithms 1 and 2, respectively. Like the original timelines, each new timeline is

a sequence of outages assigned to the same plant. However, the outages may have a newly assigned plant and a new catalyst layer decision. Using these new timelines, SCR schedule generation creates two schedules for each timeline. The method used to generate schedules is to fix the amount of NH $_3$  slip at two levels; the level that the assigned plant is currently using and the maximum allowed by the plant. Since NO $_x$  is a function of NH $_3$  and RP these two levels create two schedules per timeline of calculated NO $_x$  reduction value. One of the schedules uses the same NH $_3$  slip as the assigned plant is currently using (typically 2 ppm), while the other schedule increases the NH $_3$  slip to the maximum allowed by the plant (typically 4ppm). Finally, SCR schedule generation calculates average NO $_x$  and operating costs and returns these schedules. Table 2 shows the list of symbols used in Algorithms 1 and 2 and Figure 4 shows an overview of find timelines and generate timelines algorithms.

Table 2 Lists of symbols used in Algorithms 1 and 2

Sets and indices symbols	Descriptions
P	Set of all plants information fleet-wide as shown in Table 1
0	Set of all outages information fleet-wide as shown in Table 1
T	Set of generated timelines.
$O^+$	Set of next outage event in the timelines.
0	Each outage in the set O.
$o^1$	First outage event in the timelines.
$o^+$	Next outage event in the timelines.
$o^n$	Outage event $n$ in the timelines.
p	Each plant in the Set P
$o^1(p)$	First outage in the schedule assigned to plant <i>p</i>
τ	Each timeline in the Set <i>T</i>

# **Algorithm 1** Generate Timelines

 $\overline{\text{Let } P \text{ and } O \text{ be the}}$  sets of plants and the outages.

Let timeline set  $T = \phi$  be the set of generated timelines.

For each outage  $o \in O$  do

If outage o is the last outage of one of the original timelines then

Let outage set  $O^+(o) = \phi$ 

Else

Let outages set  $O^+(o)$  be such that each outage  $o^+ \in O^+(o)$  is such that the ending time of outage o and the starting time of outage  $o^+$  are within a predetermined window of days apart, usually around 270 to 450 days

## End if

For each plant  $p \in P$  do

Let outage  $o^1(p)$  be the first outage in the schedule originally assigned to plant p

Let timeline  $\tau = \langle o^1(p) \rangle$ 

Let timeline set  $T = T \bigcup$  Find Timelines $(\tau)$ 

End for

**Return** timeline set T

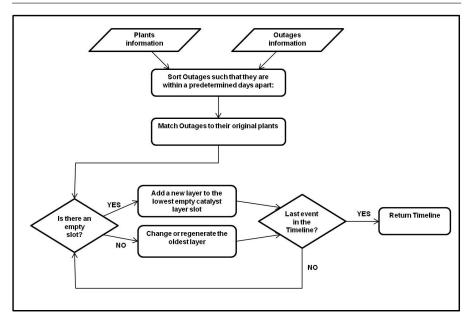


Fig. 4 An overview of Generate Timelines and Find Timelines Algorithms

# **Algorithm 2** Find Timelines( $\tau$ )

Let outage  $o^n(\tau)$  and plant  $p(\tau)$  be the last outage and the assigned plant of timeline  $(\tau)$ 

Let timeline set  $T(\tau) = \phi$  be the set of generated timelines that extend from timeline  $\tau$ 

If outage set  $O^+(o^n(\tau)) = \phi$  then

**Return** the set of timelines  $\{\tau\}$ 

Else

For each outage  $o^+ \in O^+(o^n(\tau))$  do

Let outage  $\bar{o}^+$  be a copy of outage  $o^+$  in which the assigned plant of outage  $\bar{o}^+$  is plant  $p(\tau)$  and the catalyst layer decision is to change or regenerate the oldest catalyst later at plant  $p(\tau)$  based upon timeline  $\tau$ 

Let timeline  $\bar{\tau} = \langle \tau, \bar{o}^+ \rangle$ 

Let timeline set  $T(\tau) = T(\tau) \cup \text{Find Timelines}(\bar{\tau})$ 

If there is an empty catalyst later slot at plant  $p(\tau)$  based upon the timeline  $\tau$  then

Let outage  $\hat{o}^+$  be a copy of outage  $o^+$  in which the assigned plant of outage  $\hat{o}^+$  is plant  $p(\tau)$  and the catalyst layer decision is to add a new layer to the lowest empty catalyst layer slot at plant  $p(\tau)$  based upon the timeline  $\tau$ 

Let timeline  $\hat{\tau} = \langle \tau, \hat{o}^+ \rangle$ 

Let timeline set  $T(\tau) = T(\tau) \cup \text{Find Timelines}(\hat{\tau})$ 

End if

End for

**Return** timeline set  $T(\tau)$ 

End if

## 4.3 SCR Optimization

The primary purpose of the SCR optimization module is to find an optimal set of schedules based upon the schedules generated from the SCR schedule generation module described in Section 4.2. The mathematical optimization technique applied by SCR optimization is integer linear programming while the solver uses Computational Infrastructure for Operations Research branch and cut (COIN-OR CBC [1]), which is described in this section.

Integer linear programming is a linear optimization technique in which some or all the variables are restricted to integer values. An integer programming problem in which all variables are required to be integer is called a *pure integer programming problem*. If some variables are restricted to be integer and some are not then the problem is a *mixed integer programming problem*. Problems in which the integer variables are restricted to be 0 or 1 are called pure (mixed) *0-1 programming problems* or pure (mixed) *binary integer programming problems*. In this case, the problem is a pure 0-1 programming or pure binary integer programming problem because all variables are required to be 0 or 1 [14].

The SCR optimization module finds a set of schedules that maximize  $NO_x$  emissions reduction subject to a total operating costs and power generation plan. The SCR optimization module uses an integer linear programming problem with the following:

- 1. Decision Variables: For each generated schedule, a 0-1 decision variable determines whether the schedule is used in the optimal plan.
- 2. Objective: The objective function is to maximize the anticipated average daily NO<sub>x</sub> reduction over all power plants. (The objective can be seamlessly changed to maximize the anticipated average daily reactor potential. This will reduce computationally efficiency of the tool, because average daily reactor potential has a closed-form equation, while average daily NO<sub>x</sub> reduction usually requires numerical integration. The NO<sub>x</sub> reduction equation is a concave function and has no closed-form equation.)
- 3. Constraints: The constraints of the model ensure that the optimal SCR maintenance plan maintains the following conditions:
  - The total anticipated operating costs of the plan is less than or equal to a predetermined budget.
  - The total anticipated power production is greater than or equal to a predetermined minimum production.
  - Each plant will be assigned to exactly one schedule in the plan.
  - Each outage is included in at most one schedule in the plan.

Let *S* be the set of all schedules from the SCR schedule generation module, let *P* be the set of plants, and let *O* be the set of outages. For each schedule  $s \in S$ , let  $DNOX_s$  be the NO<sub>x</sub> reduction of *s*, let  $c_s$  be the operating costs, let  $g_s$  be the power generation, and let

$$x_s = \begin{cases} 1 \text{ if schedule } s \text{ is selected for the outage,} \\ 0 \text{ otherwise.} \end{cases}$$
 (7)

For each outage  $o \in O$ , let S(o) be the schedules that include outage o, and for each plant  $p \in P$ , let S(p) be the set of schedules that can be assigned to plant p. Let

C be the maximum operating costs of the fleet, and let G be the minimum power generation. The integer linear programming problem is given by the following:

$$\max \sum_{s \in S} DNOX_s x_s \tag{8}$$

$$s.t.$$
 (9)

$$\sum_{s \in S(p)} s.t. \tag{9}$$

$$\sum_{s \in S(p)} x_s = 1 \qquad \forall p \in P \tag{10}$$

$$\sum_{s \in S(o)} x_s \le 1 \qquad \forall o \in O \qquad (11)$$

$$\sum_{s \in S} c_s x_s \le C \qquad (12)$$

$$\sum_{s \in S} g_s x_s \ge G \qquad (13)$$

$$\sum_{s} c_s x_s \le C \tag{12}$$

$$\sum_{s \in S} g_s x_s \ge G \tag{13}$$

$$x \in \{0,1\}^{|S|} \tag{14}$$

The solver within the SCR optimization module uses COIN-OR branch and cut (COIN-OR CBC). Branch and cut first achieved success in solving large instances of the traveling salesman problem [15]. It is the core of the fastest commercial general purpose integer programming packages. It is like branch-and-bound, except that in addition, the algorithm may generate cutting planes [14]. These cutting planes are constraints that, when added to the problem at a search node, result in a tighter LP polytope (while not cutting off the optimal integer solution) and thus generate a higher lower bound. The higher lower bound in turn can cause earlier termination of the search path, and thus yields smaller search trees. COIN-OR CBC is an open-source mixed integer programming solver also written in C++. The following are some basic parameter settings within CBC which could potentially increase the speed of the solver.

- 1. Cutoff: cutoff all nodes with objective greater than or less than a specified value.
- 2. IntegerTolerance: treat variables as integer if close enough.
- 3. Seconds: treat as maximum nodes after this time.
- 4. CutDepth: only generate cuts at multiples of this.
- 5. MaxNodes: stop after this many nodes.
- 6. PassCuts: number of cut passes at root.
- 7. StrongBranching: number of candidates for strong branching.

COIN-OR CBC uses strong branching where the algorithm performs a one-step look ahead for each variable that is non-integral in the LP at the node. The one-step look ahead computations solve the LP relaxation for each of the children.

The SCR management tool employs the SCR optimization module multiple times to determine an efficient Pareto optimal frontier. This Pareto optimal model provides a tradeoff between NO<sub>x</sub> reduction and operating costs. The model calculates multiple outage plans, or *Pareto points*, that are not dominated by any other outage plan in operating costs and NO<sub>x</sub> reduction. Users input a minimum and maximum budget interval, and the number of Pareto points to be determined. For instance, suppose the number of Pareto points is three, and the minimum budget is \$2 million, while the

maximum budget is \$4 million. The SCR management tool will find three outage plans that maximize  $NO_x$  reduction and have operating costs of no more than \$2 million, \$3 million, and \$4 million.

#### 5 Computational Experiments

In this section we discuss two example problem instances. The instance in Section 5.1 has seven power plants, and the instance in Section 5.2 includes six power plants. Both cases use a five-year planning horizon with approximately one layer either being added or changed each year which is a typical maintenance interval. The values are based upon default settings in CatReact [9]. In these two instances, we have decided to maximize the  $NO_x$  reduction. Although from the global information in Table 1, the fleet-wide constraints include both minimum  $NO_x$  reduction and minimum costs. Therefore, the objective function can also be easily changed to cost.

### 5.1 Optimization Results

Using the SCR management tool, we obtained three additional outage plans with different objectives and constraints as shown in Table 3. The original plan is the current plan in the outage.txt file. The max  $DNO_x$  plan is an outage plan that maximizes  $NO_x$  reduction without a constraint on the operating costs. The min cost plan is one that minimizes operating costs while ignoring  $NO_x$  reduction. Finally, the optimal plan was found by maximizing  $NO_x$  reduction subject to an operating budget no greater than that of the original plan. In all four plans, we maintained the same power generation plan. From Table 3, the optimal plan has a substantially higher  $NO_x$  reduction rate and a slightly smaller operating costs than the original plan. Observe that the  $NO_x$  reduction of the optimal plan is nearly that of the unconstrained max  $DNO_x$  plan. The primary reason for this dramatic improvement in  $NO_x$  reduction is likely due to elevated levels of  $NH_3$  slip from 2 ppm to 4 ppm at each of the plants.

## 5.2 Pareto Optimal Efficient Frontiers

We obtained a six-plant example that included outages over 5 years. The low budget used was \$67 million while the high budget was \$117 million. We did a preliminary analysis before hand and found those intervals were appropriate because the lowest possible operating cost is \$67.37 million, which is why the first point does not show any results. Similarly for the high budget, we found that no matter how much the budget is increased, the best solution that is possible to obtain is an outlet  $NO_x$  reduction of 2840.28 lbs/hr. The number of Pareto points was set to 20. The results are summarized Table 4. A plot of the Pareto optimal efficient frontier from Table 4 is given in Figure 5. From Figure 5, we can observe a large change in  $NO_x$  reduction from 2626.52 lbs/hr to 2767.1 lbs/hr with an increase in operating costs of roughly \$4 million. This graph is very helpful since it would allow users to find the trade off of increasing operating costs to further reduce  $NO_x$ .

Table 3  $NO_x$  reduction and operating costs of four outage plans

Outage Plan	Plant Number	NO <sub>x</sub> Reduction (%)	Operating Costs (\$million)
	Plant 1	78.06	50.61
	Plant 2	92.53	56.46
	Plant 3	77.79	50.62
Original Plan	Plant 4	84.50	53.70
	Plant 5	79.29	51.16
	Plant 6	78.40	50.61
	Plant 7	74.29	53.33
	Total	80.69	366.49
	Plant 1	96.32	53.79
	Plant 2	97.10	56.46
	Plant 3	96.29	53.81
Max DNO <sub>x</sub> Plan	Plant 4	96.37	53.81
	Plant 5	98.05	54.32
	Plant 6	96.50	53.80
	Plant 7	90.73	56.50
	Total	95.91	382.49
Min Cost Plan	Plant 1	77.26	50.58
	Plant 2	81.35	53.37
	Plant 3	75.93	50.58
	Plant 4	74.94	50.58
	Plant 5	73.83	38.26
	Plant 6	72.15	51.15
	Plant 7	67.23	40.48
	Total	74.69	335.01
Optimal Plan	Plant 1	96.11	50.58
	Plant 2	97.11	56.64
	Plant 3	96.06	53.81
	Plant 4	96.17	53.81
	Plant 5	97.77	54.26
	Plant 6	96.35	53.80
	Plant 7	89.34	43.04
	Total	95.56	365.94

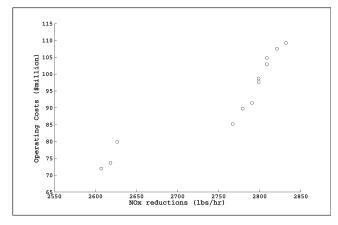


Fig. 5 Pareto optimal efficient frontiers of operating costs vs. NO<sub>x</sub> reduction

Table 4 Pareto optimal plans

Pareto Points	Budget (\$)	NO <sub>x</sub> Reduction (lbs/hr)	Operating Costs (\$)
1	67000000		
2	69631600	2594.94	67367800
3	72263200	2607.11	71942200
4	74894700	2618.3	73657600
5	77526300	2618.3	73657600
6	80157900	2626.52	79870800
7	82789500	2626.52	79870800
8	85421100	2767.1	85149000
9	88052600	2767.1	85149000
10	90684200	2779.27	89723400
11	93315800	2790.46	91438800
12	95947400	2790.46	91438800
13	98578900	2798.68	97652000
14	101211000	2798.68	98704200
15	103842000	2808.7	102930000
16	106474000	2808.7	104760000
17	109105000	2820.87	107505000
18	111737000	2832.06	109220000
19	114368000	2832.06	109220000
20	117000000	2840.28	116485000

#### 6 Conclusion and Future Directions

In this paper, we developed a mathematical optimization technique for managing a fleet of plants using SCR technology as opposed to a single unit. For future research, we will focus on improving the algorithm performance. As stated earlier, the SCR management framework consists of two modules, which are SCR schedule generation and SCR optimization. The SCR schedule generation currently generates all possible schedules using enumeration, which is clearly the bottleneck of the tool. We can likely improve the computational efficiency of the algorithm by integrating schedule generation and optimization in a branch-and-price approach.

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# References

- 1. COIN-OR Branch-and-Cut MIP Solver. https://projects.coin-or.org/Cbc
- 2. Tennessee Valley Authority: Coal-fired power plant. http://www.tva.gov/power/coalart.htm
- 3. The U.S. Department of Energy and Southern Company Services, Inc.: Topical report number 9, control of nitrogen oxide emissions: Selective catalyst reduction (SCR). http://www.netl.doe.gov/technologies/coalpower/cctc/topicalreports/pdfs/topical9.pdf (1997)
- 4. Chen, J., Frey, H.: Optimization under variability and uncertainty: A case study for NOx emissions control for a gasification system. Environmental Science and Technology 38, 6741–6747 (2004)
- Cichanowicz, J., Muzio, L.: Factors affecting selection of a catalyst management strategy. In: Proceedings of the DOE-EPRI-EPA-AWMA Power Plant Air Pollutant Control Mega Symposium: DOE/EPRI/EPA/AWMA. Washington, DC (2003)

- Cichanowicz, J., Smith, L., Muzio, L.: Twenty-five years of SCR evolution: Implications for U.S. application and operation. In: Proceedings of the EPRI-DOE-EPA Combined Power Plant Air Pollutant Control Symposium: The MEGA Symposium; EPRI/DOE/EPA. Chicago, IL (2001)
- Cichanowicz, J., Smith, L., Muzio, L., Marchetti, J.: 100 gw of SCR: Installation status and implications of operating performance on compliance strategies. In: Proceedings of the EPA-EPRI-NETLAWMA Combined Power Plant Air Pollutant Control Mega Symposium: EPA/EPRI/NETL/AWMA. Washington, DC (2003)
- 8. Diwekar, U., Rubin, E., Frey, H.: Optimal design of advanced power systems under uncertainty. Energy Conversion and Management **38**(15), 1725–1735 (1997)
- 9. FERCo: CatReact software. http://www.ferco.com/catreact.html
- Frey, H.: Engineering-economic evaluation of SCR NOx control systems for coal-fired power plants.
   In: Proceedings of the American Power Conference. Chicago, Illinois (1995)
- 11. Grabitech: MultiSimplex software. http://www.grabitech.com/Multisimplex.htm
- 12. Mi, J.: CFD for SCR design. Tech. rep., Southern Company Inc.
- Muzio, L., Quartucy, G., Cichanowicz, J.: Overview of status of post-combustion NOx control: SNCR, SCR, and hybrid technologies. International Journal of Environment and Pollution 17(1-2), 4–30 (2002)
- 14. Nemhauser, G., Wolsey, L.: Integer and combinatorial optimization. Wiley-Interscience (1999)
- 15. Padberg, M., Rinaldi, G.: A branch-and-cut algorithm for the resolution of large-scale symmetric traveling salesman problems. SIAM Rev. **33**(1), 60100 (1991)
- 16. Pritchard, S., DiFrancesco, C.: SCR catalyst management: Enhancing operational flexibility. Tech. rep., Cormetech, Inc. (2006)
- Pritchard, S., DiFrancesco, C., Kaneko, S., Kobayashi, N., Suyrgama, K., Eda, K.: Optimizing SCR catalyst design and performance for coal-fired boilers. In: Proceedings of the EPRI/EPA 1995 Joint Symposium on Stationary Combustion NO Control. Kansas City, MO (1995)
- Rogers, K., Milobowski, M., Wooldridge, B.: Perspectives on ammonia injection and gaseous static mixing in SCR retrofit applications. In: Proceedings of the EPRI-DOE-EPA Combined Utility Air Pollutant Control Symposium. Atlanta, Georgia (1999)
- Rubin, E., Kalagnanam, J., Frey, H., Berkenpas, M.: Integrated environmental control concepts for coal-fired power plants. Journal of the Air and Waste Management Association 47(11), 1180–1188 (1997)
- Rubin, E., Salmento, J., Frey, H.: Cost-effective emission controls for coal-fired power plants. Chemical Engineering Communications 74, 155–167 (1988)
- Staudt, J., Engelmeyer, A.: SCR catalyst management strategies-modeling and experience. In: Proceedings of the DOE-EPRI-EPA-AWMA Power Plant Air Pollutant Control Mega Symposium: DOE/EPRI/EPA/AWMA. Washington, DC (2003)