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Synthesizing Optimal Waste Blends

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Abstract

Vitrification of tank wastes to form glass is a technique that will be used for the disposal of high-level waste at Hanford. The amount of glass produced can be reduced by blending of the wastes. The optimal way to combine the tanks to minimize the volume of glass can be determined from a discrete blend calculation. However, this problem results in a combinatorial explosion as the number of tanks increases. Moreover, the property constraints make this problem highly non-convex where many algorithms get trapped in local minima. In this paper we examine the use of different combinatorial optimization approaches to solve this problem. A two stage approach using a combination of Simulated Annealing and nonlinear programming (NLP) is developed. The results of different methods such as heuristics approach based on human knowledge and judgment, mixed integer nonlinear programming (MINLP) approach with GAMS, and branch and bound with lower bound derived from the structure of the given blending problem are compared with this coupled Simulated Annealing and NLP approach.
Keywords: Blending, Waste Disposal, Branch and Bound, Simulated Annealing.

1 Introduction

The Hanford Site in southeastern Washington produced nuclear materials using various processes for nearly fifty years. Radioactive waste was produced as by-products of the processes. This waste will be retrieved and separated into high-level and low-level portions. The high-level and low-level wastes will be immobilized for future disposal.

The high-level waste will be converted into a glass form for disposal. The glass must meet both processibility and durability restrictions. The processibility conditions ensure that during processing the glass melt has properties such as viscosity, electrical conductivity and liquidus temperature that lie within ranges known to be acceptable for the vitrification process. Durability restrictions ensure that the resultant glass meets the quantitative criteria for disposal in a repository. There are also bounds on the composition of the various components in the glass. In the simplest case, waste and appropriate glass forms (frit) are mixed and heated in a melter to form a glass that satisfies the constraints. It is desirable to keep the amount of frit added to a minimum for two reasons. First, this keeps the frit costs to a minimum. Second, the amount of waste per glass log formed is maximized and this keeps the waste disposal costs to a minimum. When there is only a single type of waste the problem of finding the minimum amount of frit is relatively easy.

Hanford has 177 tanks (50,000 to 1 million gallons) containing radioactive waste. Since these wastes result from a variety of processes, these wastes vary widely in composition, and the glasses produced from these wastes will be limited by a variety of components. The minimum amount of frit would be used if all the high-level wastes were combined to form a single feed to the vitrification process. Because of the volume of waste involved and the time span over which it will be processed, this is logistically impossible. However, much of the same benefit can be obtained by forming blends from sets of tanks. The problem is how to divide all the tanks into sets to be blended together such that the minimal amount of frit is required.

2 Problem Description

In this discrete blending problem, there are *N* different sources of waste which have to form a discrete number of blends *B*, the number of blends being less than the number of sources or tanks. All the waste from any given tank are required to go to a single blend and each blend contains waste from *N/B* sources. Blends of equal size (same number of wastes per blend) were specified; alternatively, blends could be formulated to have approximately the same waste masses. If neither of these were constrained, all the waste would go to a single blend. The basic glass formulation problem was described in Hoza (1994).

Let N be number of wastes, B be number of blends, and T be number of wastes per blend. Therefore, $T = N/B$. Frit is added to each of these blends to form glass of particular quality. If $w^{(i)}$ is the mass of i-th component in the waste, $f^{(i)}$ is the mass of i-th component in the frit and $g^{(i)}$ is th mass of i-th component in the glass (where total mass of glass is given by G), which results in the equality constraints: (1) $g^{(i)} = w^{(i)} + f^{(i)}$, (2) $G = \sum_{i=1}^{n} g^{(i)}$, and (3) $fg^{(i)} = g^{(i)}/G$. Where n is the total number of chemical components and $fg^{(i)}$ denotes the fraction of i-th component in the glass.

In order to form glass the blend must satisfy certain constraints. These constraints are briefly described below.

1. **Individual Component Bounds:** There are upper ($fg_{UL}^{(i)}$) and lower ($fg_{LL}^{(i)}$) limits on the fraction of each component in glass. Therefore, $fg_{LL}^{(i)} \leq fg^{(i)} \leq fg_{UL}^{(i)}$.
2. **Crystallinity Constraints:** The crystallinity constraints or multiple component constraints specify the limits on the combined fractions of different components. There are five such constraints.
3. **Solubility Constraints:** These constraints limit the maximum value for the mass fraction of one or a combination of components.
4. **Glass Property Constraints:** These constraints govern the properties of viscosity, electrical conductivity and durability.

Blending is most effective when the limiting constraint is one of the first three types. In these cases, one, or a small number of components is limiting. The compositions of these components vary widely in the wastes, so blending averages out the limiting species, resulting in a better overall solution requiring less frit.

If there was only one blend then the problem is relatively straight forward non linear programming problem (NLP) with a linear objective and a mix of linear and quadratic constraints. The objective is to: $Min \sum_{i=1}^{n} f^{(i)}$.
Subject to: *Equality constraints (given above), Individual component bounds, Crystallinity constraints, Solubility constraints, and Glass property constraints.*

The problem is complicated by the presence of a set of wastes which need to be partitioned to form blends. Frit is added to each of the blends to form glass. Since the composition is different in each blend, the manner in which the waste set is partitioned affects the amount of frit and the composition of the frit which needs to be added.

The objective in this phase is to select the combination of blends so that the total amount of frit used is minimized. The number of possible combinations is given by the formula: $\frac{N!}{B!(T!)^B}$.

We have selected 21 tanks for this study to be partitioned into 3 blends. The information about chemical composition and amount of waste in each tank was obtained from the unpublished material provided by one of the authors. From the above formula, for a problem with 21 wastes with to be partitioned into 3 blends, there are 66512160 possible combinations to examine. Clearly examining all possible combinations is a very onerous task and nearly impossible for larger problems. We therefore have to resort to either a heuristic approach or use combinatorial optimization methods like mathematical programming techniques or probabilistic combinatorial methods like Simulated Annealing.

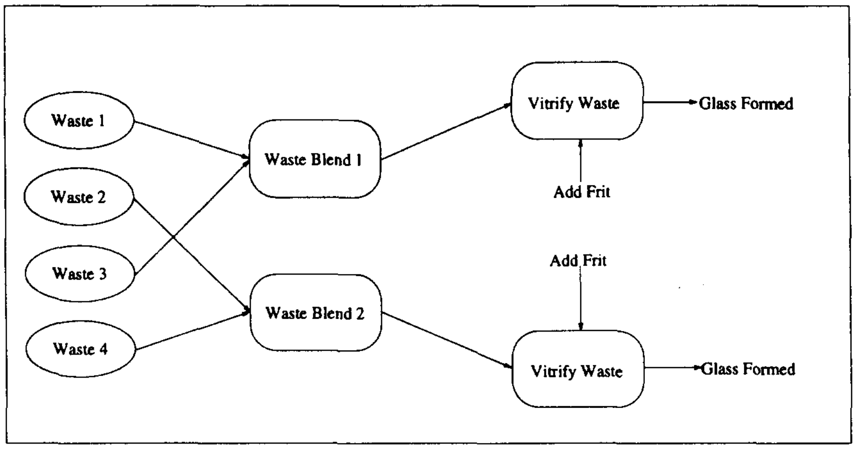

Figure 1: Conversion of Waste to Glass

3 Solution Methods

The state of the art combinatorial optimization techniques which can be used for the solution of the optimal waste blending problems include: a) the mathematical programming approach which involves use of Mixed Integer Nonlinear Programming (MINLP) algorithms, b) the heuristic approach which relies on intuition and engineering knowledge, and c) an approach based on use of probabilistic optimization methods like Simulated Annealing.

In this paper we explore the use of the above mentioned three approaches to solve this problem. For this study twenty one tanks were chosen which needs to form three blends. At first, the problem was formulated and implemented in General Algebraic Modeling Systems (GAMS) (Brooke et al., 1992). GAMS uses the outer approximation/equality relaxation/augmented penalty function, OA/ER/AP (Viswanathan and Grossmann, 1990) algorithm for the solution of MINLP problems. While, this algorithm is computationally efficient, due the non-convex nature of constraints it fails to find the global optimum. A branch and bound procedure using the structure of the problem was also developed. This algorithm reached global optimum but was computationally intensive. The heuristic approach could get to a solution reasonably close to global optimum but was again restricted to this particular problem only. A two-stage approach involving combination of Simulated Annealing and nonlinear programming algorithms led to the global optimal solution in a reasonable amount of time.

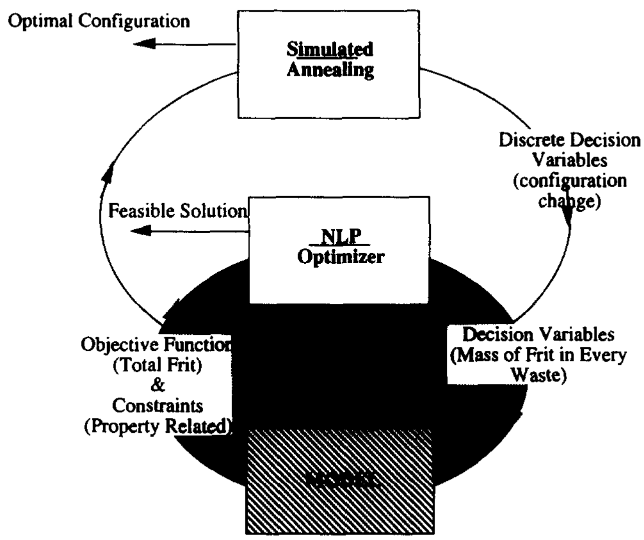

Figure 2: Optimum Discrete Blending Problem: Solution Procedure

Heuristic Approach In a heuristic approach to solving the discrete blending problem, we first determined the limiting constraint for a total blend of all tanks being considered (twenty-one, in this case). Then we tried to formulate blends such that all blends have the same limiting constraint. If this can be achieved, the frit required would be the same as for the total blend. This approach, however, was very difficult to implement; rather, we formulated blends to try to ensure that all blends were near the limiting value for the limiting constraint. Using this approach, the best solution obtained was 11,735.96 kgs of frit.

GAMS-based MINLP Approach The GAMS based MINLP solution was very dependent on the starting conditions for the calculation. The conditions specified were the initial distribution of each tank among the blends (for the relaxed initial optimization) and the frit composition of each of the blends. The best MINLP solution was 12,341.69 kgs of frit. The GAMS based MINLP model failed to find the global optimal solution because the problem is highly nonconvex with the presence of several bilinear constraints.

For the particular problem in hand we also developed branch and bound procedure. Since this procedure was specific to the three blend problem and also computationally intensive, it was used to check the global optimality of the Simulated Annealing solution procedure. Hence, it is presented after the Simulated Annealing solution procedure.

The Coupled Simulated Annealing-NLP Approach The optimal waste loading problem which we have addressed here is the discrete blending problem, where amount of frit required to meet the various constraints is minimized by blending optimal configurations of tanks and blends. We have used a 2 loop solution procedure based on Simulated Annealing and nonlinear programming. In the inner loop nonlinear programming (NLP) is used to ensure constraint satisfaction by adding frit. In the outer loop the best combination of blends is sought using Simulated Annealing so that the total amount of frit used is minimized. Figure 2 shows the schematic of this procedure used for solving the discrete blend problem.

The analogy in Simulated Annealing is to the behavior of physical systems in the presence of a heat bath: in physical Annealing, all atomic particles arrange themselves in a lattice formation that minimizes the amount of energy in the substance, provided the initial temperature(T_{init}) is sufficiently high and the cooling is carried out slowly. At each temperature T, the system is allowed to reach thermal equilibrium, which is characterized by the probability (Pr) of being in a state with energy E given by the Boltzmann distribution:$Pr_E = \frac{1}{Z_t} e^{\frac{-\Delta E}{K_b T}}$, where K_b is Boltzmann's constant ($1.3806 \times 10^{23}\ J/degreesK$) and $\frac{1}{Z_t}$ is a normalization factor (Collins et al. 1988).

A major difficulty in application of Simulated Annealing is defining the analog to the entities in physical Annealing. Specifically, it is necessary to specify the following: the objective function, the configuration space and the move generator, and the temperature schedule. All of the above are dependent on the problem structure. So for the discrete blending problem we use the following specifications.

The objective for SA is – Minimize total mass of frit used over a given combination of blends i.e.

$$Min \sum_{j=1}^{B} \sum_{i=1}^{n} f_j^{(i)}$$

Configuration Space and the Move Generator: Consider the problem where we have 21 wastes (indexed by 1, 2, . . . , 21) and we wish to form 3 blends with these wastes. Our objective is to find the best combination of blends. Suppose an initial state is such that: Blend 1 = [1 2 3 4 5 6 7]; Blend 2 = [8 9 10 11 12 13 14]; Blend 3 = [15 16 17 18 19 20 21]. A neighbor to this state can be defined as the state which can be reached by the application of a single operator. For a problem with 3 blends we can devise 3 simple operators:(1) Swap(1,2) - where we swap elements between Blend 1 and Blend 2 (1/3 probability), (2) Swap(2,3) - where we swap elements between Blend 2 and Blend 3 (1/3 probability), and (3) Swap(1,3) - where we swap elements between Blend 1 and Blend 3 (1/3 probability).

We need two more operators to decide which two elements from the two blends are to be swapped. For these studies we have kept equi-probable chance for one of the seven elements to be chosen from each of the two blends.

Temperatures Schedule: If the initial temperature is too low, the search space is limited and the search becomes trapped in a local region. If the temperature is too high, the algorithm spends a lot of time jumping around wasting CPU time. A rule of thumb for this is to select an initial temperature where a high percentage of moves are accepted. We have chosen 1000 as the initial temperature. The final temperature is chosen so that the algorithm terminates after 10 successive temperature decrements with no change in the optimal state. Choosing the temperature decrement is also rather tricky. If the temperature decrement is too big, the algorithm quickly "quenches" and could get stuck in a poor local optima. On the other hand, if the temperature decrement is too small excessive computational effort is required. A very simple rule which may be used is: $T_{new} = \alpha T_{old}$, where $0.8 \leq \alpha \leq 0.99$. We have chosen α to be 0.95.

The Optimal Solution:The Simulated Annealing procedure provided a solution of 11028.43 (kgs of frit) which we were able to later confirm to be the global optimum using a branch and bound procedure. The composition of the blends was as follows: Blend 1 [Tanks] = [20 3 9 4 8 6 5], Blend 2 [Tanks] = [21 12 11 10 19 16 1], and Blend 3 [Tanks] = [17 15 14 2 18 13 7].

In order to find a guaranteed optimal solution every combination of wastes must be examined. The enumerative procedure is also composed of two procedures as for each of the possible blend combinations the amount of frit required for each blend must be found by the NLP. The outer loop is an enumerative procedure which supplies the inner loop the wastes which might be combined to form a blend. In the inner loop an NLP informs the outer loop about the amount of frit necessary to form glass. While this method finds a guaranteed optimal solution, unfortunately the number of possible combinations we need to examine grows exponentially in the number of wastes available.

As mentioned before, the test problem with 21 wastes to be partitioned into 3 blends has 66512160 possible combinations to examine. The number of combinations that must be *explicitly* examined to verify optimality can be reduced by using a branch and bound method. The initial configuration is used as the starting *upper bound*. In the case of the test problem the *lower bound* can be obtained in the following manner:

1. Fix the wastes for the first blend and calculate the amount of frit.
2. Relax the requirement that the remaining wastes must form two blends and assume that they form a single blend. Now calculate the amount of frit required for this relaxation.
3. The total of the frit for the first blend and the relaxation is now a valid lower bound on the original problem.

Clearly, if the lower bound is greater than the current best upper bound then any combination where the composition of one of the blends is the same as that of the first blend cannot be optimal. All these combinations can be eliminated and can be considered to be *implicitly* examined. This bounding method was sufficiently strong enough for us to solve the test problem to optimality. However, it still took about 3 days of computation (on DEC-ALPHA 400 machine) as compared to average 45 minutes of CPU time using the two-stage Annealing approach. The branch and bound procedure can be implemented using different strategies. We implemented the procedure using a *depth-first* strategy because of its minimal memory requirements. The depth-first strategy is also relatively easy to implement as a recursive function.

4 Conclusions

The purpose of this research was to develop a method which would help to decide which combination of wastes would minimize the amount of frit needed to convert the waste into glass. The benefit of reducing the amount of frit used is in reduced material costs and the reduced bulk of the glass formed which in turn reduces the disposal costs. The search space grows exponentially with an increase in parameters defining the problem, making it almost impossible to find optimal solutions for realistically sized problems. We compared different combinatorial optimization techniques such as GAMS-based MINLP algorithm, branch and bound, and Simulated Annealing and heuristics approach to find the optimal solution. We have found that a two-stage approach combining Simulated Annealing and NLP algorithms is a cost effective means to obtain global optimal or near global optimal solutions with reasonable amounts of computational effort. Both the heuristic approach and GAMS based MINLP result in local minimum. Branch and bound procedure leads to global optimum but requires significantly large computational efforts compared to the coupled Simulated Annealing-NLP approach.

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