Name:

Model-based Decision Support

Exam 5 (home assignment)

Till May 23, 2019

Blending Problems and Combinatorial Optimization: The Hanford site in South-Eastern Washington (US West coast) has produced nuclear materials using various processes for nearly 50 years. Radioactive hazardous 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 (vitrification).

http://komonews.com/news/local/hanford-on-pace-to-turn-radioactive-waste-into-glass-by-2022

https://www.youtube.com/watch?v=79pmZVz5pmI

The 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 within ranges known to be acceptable for the vitrification (glass-building) process. Durability restrictions ensure that the resultant glass meets the quantitative criteria for disposal in a repository. There are also bounds on the compositions of the various components in the glass. In the simplest case, waste and appropriate glass forming materials (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 amount of frit costs to a minimum. Second, the amount of waste per glass log formed is to be maximized, which 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 (it is a blending problem).

However, Hanford has many tanks. Consider 21 Tanks (50K to 1M litres) containing radioactive waste that should be vitrified. Because 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. Table 1 shows an example of three tanks; especially it shows the chemical composition of the waste.

		Fractional Composition of Wastes			
components / Tank ID		AY-102	AZ-101	AZ-102	W^i
SiO2 (silicon dioxide)	1	0,072	0,092	0,022	11,18365
B2O3 (boron oxide)	2	0,026	0	0,006	2,416554
Na2O	3	0,105	0,264	0,12	34,19368
Li2O	4	0	0	0	0
CaO (quicklime)	5	0,061	0,012	0,01	5,56847
MgO	6	0,04	0	0,003	2,822121
Fe2O3	7	0,328	0,323	0,392	89,00615
Al2O3	8	0,148	0,157	0,212	45,66483
ZrO2	9	0,002	0,057	0,063	11,47892
Other	10	0,217	0,096	0,173	41,71802
Total		**0,999**	**1,001**	**1,001**	244,0524
Cr2O3	11	0,016	0,007	0,005	1,95795
F	12	0,006	0,001	0,001	0,542788
P2O3	13	0,042	0,001	0,021	5,56952
SO3	14	0,001	0,018	0,009	2,080857
Noble Metals	15	0	0	0	0
Mass (unit tons)		59,772	40,409	143,747	243,928

Table 1: Glass forming materials and some problematic materials like flour (F)

Table 1 shows the waste mass expressed as a total of the first ten chemicals, including the mostly uncertain “chemical mixture” termed as “Other.” The waste mass is scaled down by 1000, let say the units are tons. In the table, the chemicals are expressed as the fraction of the total mass of the corresponding tank (tanks are labelled AY-102, AZ-101 etc.). The full information for all 21 Tanks you’ll find in an extra GAMS file. Additionally it should be mentioned that the substances Cr203, F, P203, S03, and Noble Metals are known (measured) components of **Other**: these substances represent only a small amount of **Other** but have a huge impact on the vitrification process. Other substances of Other (like water) are uncritical. Note that Cr203, Flour (F) etc. are not extra components, but they are aggregated in **Other**.

Frit added to a blend of tanks consists of the first nine chemicals or something else like water (the latter one are formally added to Other frit). Of course, the frit Other is not polluted by Cr203, F, etc. 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 21 tanks into sets to be blended together so that a minimum amount of frit is required. Let us assume that the 21 tanks should be combined of three groups each with 7 tanks. One decision is to group the tanks (combinatorial problem). The other decisions (for each group of tanks separately done) are the factions of i^{th} component in the glass (different for each group of tanks), i.e. variable p_i i = SiO2, B2O3 etc. (blending problems).

Details of Glass Property Constraints

NOTATION

C_1	Bound for Crystal1 – 3.0
C_2	Bound for Crystal2 – 0.08
C_3	Bound for Crystal3 – 0.225
C_4	Bound for Crystal4 – 0.18
C_5	Bound for Crystal5 – 0.18
k_{min}	Lower limit for conductivity – 18
k_{max}	Upper limit for conductivity – 50
μ_{min}	Lower limit for viscosity (PaS) – 2.0
μ_{max}	Upper limit for viscosity (PaS) – 10.0
$D_{\text{max}}^{\text{PCT}}$	Max release rate (product consistency test) (g per m_2) – 10.0
$D_{\text{max}}^{\text{MCC}}$	Max release rate (materials characterization center) (g per m^2) – 28.0
μ_a^i	Linear coefficients of viscosity model
μ_b^{ij}	Cross term coefficients of viscosity model
k_a^i	Linear coefficients of electrical conductivity model
k_b^{ij}	Cross term coefficients of electrical conductivity model
Dp_a^i	Linear coefficients of durability (PCT) model (for Boron)
Dp_b^{ij}	Cross term coefficients of durability (PCT) model for Boron
Dm_a^i	Linear coefficients of durability (MCC) model (for Boron)
Dm_b^{ij}	Cross term coefficients of durability (MCC) model (for Boron)

1. Component Bounds:

   a) $0.42 \le p^{(\text{SiO}_2)} \le 0.57$
   b) $0.05 \le p^{(\text{B}_2\text{O}_3)} \le 0.20$
   c) $0.05 \le p^{(\text{Na}_2\text{O})} \le 0.20$
   d) $0.01 \le p^{(\text{Li}_2\text{O})} \le 0.07$
   e) $0.0 \le p^{(\text{CaO})} \le 0.10$
   f) $0.0 \le p^{(\text{MgO})} \le 0.08$

g) $0.02 \leq p^{(Fe_2O_3)} \leq 0.15$
h) $0.0 \leq p^{(Al_2O_3)} \leq 0.15$
i) $0.0 \leq p^{(ZrO_2)} \leq 0.13$
j) $0.01 \leq p^{(\text{other})} \leq 0.10$

2. Five glass crystallinity constraints:

a) $p^{(SiO_2)} > p^{(Al_2O_3)} * C_1$
b) $p^{(MgO)} + p^{(CaO)} < C_2$
c) $p^{(Fe_2O_3)} + p^{(Al_2O_3)} + p^{(ZrO_2)} + p^{('Other')} < C_3$
d) $p^{(Al_2O_3)} + p^{(ZrO_2)} < C_4$
d) $p^{(MgO)} + p^{(CaO)} + p^{(ZrO_2)} < C_5$

3. Solubility Constraints:

a) $p^{(Cr_2O_3)} < 0.005$
b) $p^{(F)} < 0.017$
c) $p^{(P_2O_5)} < 0.01$
d) $p^{(SO_3)} < 0.005$
e) $p^{(Rh_2O_3+PdO+Ru_2O_3)} < 0.025$

4. Viscosity Constraints:

a) $\sum_{i=1}^{n} \mu_a^i * p^{(i)} + \sum_{j=1}^{n} \sum_{i=1}^{n} \mu_b^{ij} * p^{(i)} * p^{(j)} > \log(\mu_{\min})$
b) $\sum_{i=1}^{n} \mu_a^i * p^{(i)} + \sum_{j=1}^{n} \sum_{i=1}^{n} \mu_b^{ij} * p^{(i)} * p^{(j)} < \log(\mu_{\max})$

5. Conductivity Constraints:

a) $\sum_{i=1}^{n} k_a^i * p^{(i)} + \sum_{j=1}^{n} \sum_{i=1}^{n} k_b^{ij} * p^{(i)} * p^{(j)} > \log(k_{\min})$
b) $\sum_{i=1}^{n} k_a^i * p^{(i)} + \sum_{j=1}^{n} \sum_{i=1}^{n} k_b^{ij} * p^{(i)} * p^{(j)} < \log(k_{\max})$

6. Dissolution rate for boron by PCT test (DissPCTbor):
$\sum_{i=1}^{n} Dp_a^i * p^i + \sum_{j=1}^{n} \sum_{i=1}^{n} Dp_b^{ij} * p^{(i)} * p^{(j)} < \log(D_{\max}^{PCT})$
7. Dissolution rate for boron by MCC test (DissMCCbor):
$\sum_{i=1}^{n} Dm_a^i * p^i + \sum_{j=1}^{n} \sum_{i=1}^{n} Dm_b^{ij} * p^{(i)} * p^{(j)} < \log(D_{\max}^{MCC})$

Table 2: In order to form glass, a blend must satisfy certain "strict standards"

Additionally we use some auxiliary decisions variables like

- "amount of component i originally in the blend (group of tanks) $W^{(i)}$ "¸ it should be obvious that $W^{(i)}$ is computed with data like in Table 1. It is variable, because if one changes the tank composition of a group (blend), obviously $W^{(i)}$ changes, too.
- " mass of the i^{th} component in the frit ($f^{(i)}$) ", amount of glass building component i added.
- " mass of i^{th} component in the glass (blend) $g^{(i)}$ " -- $g^{(i)}$ results from the sum of $f^{(i)}$ and $W^{(i)}$,
- " the total mass of the blend G "; G is the sum of the $g^{(i)}$ (of course done for every group of tanks).
- $f^{(i)}$ relates to $p^{(i)}$ via G (p = g/G), to be more precisely $p^{(i)} = (f^{(i)} + W^{(i)}) / G$

I have provided a GAMS file at TISS where the declaration part and the coded model are already implemented. Solve this problem using a Mathematical Programming solver (keep in mind that due to the size of the problem a single optimization run may last a little bit longer) and describe the results partly in tables and partly verbally. Please add the name of the solver that you have used and how long the computation has lasted (in seconds).

Next add constraints that the total mass of a group of tanks (waste plus frits) is not **three times** as much as the mass of any of the two other groups of tanks. Report the results of this extended problem. The deadline for this home assignment is Thu May 23rd, 2019.