Manufacturing thickeners

A project in Applied Optimization

5th January 2007

1 Introduction

One of the purposes of this course is to get some practice in describing relevant parts of a real-world problem in a mathematical model. This project aids in fulfilling this purpose.

The project consists of two parts, where modeling a problem is the first part and finding and analyzing the optimal solution is the second.

In the first part, we want you to formulate a mathematical model that is linear and continuous. From the theory we know that linear, continuous problems are easy to solve. Another advantage of linear programming models is that they are quite easy to understand for people with basic knowledge of mathematics.

In the second part, you will get some experience with an optimization tool, AMPL/CPLEX, a program that is used to find and analyze the optimal solutions to linear and integer programs. The problem will be solved and some sensitivity analysis will be done.

The idea behind the project model originates in the report, Economic Analysis of Air Pollution Regulations: Miscellaneous Cellulose Manufacturing Industry (by R.H. Beach, G.L. Van Houtven, M.C. Buckley, and B.M. Depro, 2000). All company names and most of the data, however, is fictitious.

Below, Section 2 gives a short introduction to the cellulose manufacturing industry in general, to give you some background knowledge. Section 3 contains the information you need for this project. The fictitious company Aditiva's production process is described here, including chemical reactions, the raw materials, the different drying methods used, and the demands. All necessary data are given, such as prices, capacities, demand data etc. Section 4 finally contains the first part of the assignment. After a correct model is handed in and approved, in time(!), you may start with the second part, the analysis.

2 Cellulose manufacturing industry

Cellulose is a natural polymer found in plant cell walls. Figure 1 below shows the structure of the cellulose molecule. The figure shows part of a cellulose molecule, with 5 glucose units linked together. Observe that other units are linked to the chain in the same manner, both in the upper right and the lower left part of the picture. A cellulose molecule is made from about 300-10 000 of these glucose units; how many is depending on the plant.

The cellulose extracted from trees or other plants provides the basic material for all of the commercial products produced by the miscellaneous cellulose manufacturing industry.

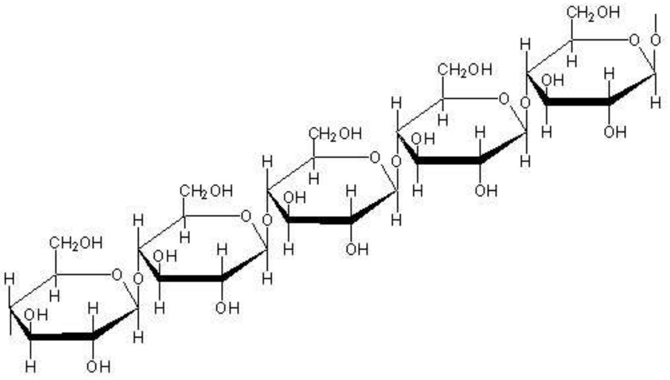

Figure 1: Cellulose is a polymer made from glucose. It is made from β-glucose units and the polymer molecules are 'straight'.

The miscellaneous cellulose manufacturing industry can be divided into two major categories: the viscose category and the cellulose ether category. Both of these categories use some type of cellulose as the primary raw material, normally either wood pulp or cotton liners, but their production processes differ. In this project only the manufacturing of cellulose ethers is considered.

Various cellulose ethers can be produced, including methyl cellulose (MC), ethyl cellulose (EC), carboxymethyl cellulose (CMC), hydroxyethyl cellulose (HEC), hydroxypropyl cellulose (HPC), and hydroxypropyl methyl cellulose (HPMC). Most of these products are in powder form, with different particle sizes.

Cellulose ethers are used as input into a variety of goods. They are mainly used as thickeners, viscosifiers, and binders in food, and in the pharmaceutical, paper, cosmetic, adhesive, detergent, and textile industries. They are also used in producing paints, personal care products, inks, and industrial coatings.

2.1 Cellulose Ether Production Process

The production of cellulose ethers demands cellulose in powder form, hence the cellulose pulp is shredded into the wanted size. The cellulose is then reacted with a sodium hydroxide (NaOH) solution to produce alkali cellulose. The NaOH breaks up the cellulose pulp by adding a hydroxide ion to the cellulose chain. This step creates a site to add constituent groups (e.g. methyl,

ethyl, or propyl groups). Following the production of alkali cellulose, the raw materials used in the cellulose ether process vary according to the particular ether being produced.

To produce MC, EC, CMC, HEC and HPC, alkali cellulose is reacted with methyl chloride, ethyl chloride, chloroacetic acid, ethylene oxide and propylene oxide, respectively. HPMC is produced by reacting alkali cellulose with both methyl chloride and propylene oxide.

In other words: all cellulose ether processes include the following steps:

1. production of alkali cellulose from cellulose and NaOH;
2. reaction of the alkali cellulose with chemical compound(s) to produce a cellulose ether product;
3. washing and purification of the cellulose ether product, and
4. drying of the cellulose ether product.

3 The Company Aditiva

3.1 Introduction

Aditiva is a company that produces cellulose ethers in the Gothenburg area. Mainly two types of thickeners are manufactured: methyl cellulose (MC) and ethyl cellulose (EC).

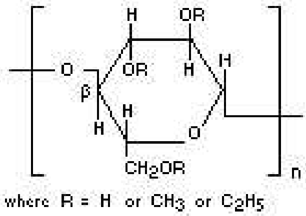

Figure 2: R = CH_3 (methyl) gives methyl cellulose and R = C_2H_5 (ethyl) gives ethyl cellulose.

Since the cellulose molecules have OH-groups, marked R in Figure 2, where sodium hydroxide can react, we below write cellulose as CelluloseOH, when we discuss the chemical reactions.

3.2 Reactions

The reactions taken place in Aditiva's reactors can be simplified as follows. When sodium hydroxide is added to the reactor, it directly goes into ions, Na^+ and OH^-.

Each of these hydroxide ions, OH^-, immediately reacts with a OH-group on the cellulose molecule CelluloseOH, producing alkali cellulose CelluloseO^- and water. This step is common in producing MC and EC, according to Reactions (1) and (3).

Further the ion CelluloseO^- reacts with methyl chloride (MetCl) or ethyl chloride (EtCl), Reactions (2) and (4).

$$\text{CelluloseOH} + \text{OH}^- \longrightarrow \text{CelluloseO}^- + \text{H}_2\text{O} \tag{1}$$
$$\text{CelluloseO}^- + \text{MetCl} \longrightarrow \text{methyl cellulose} + \text{Cl}^- \tag{2}$$

$$\text{CelluloseOH} + \text{OH}^- \longrightarrow \text{CelluloseO}^- + \text{H}_2\text{O} \tag{3}$$
$$\text{CelluloseO}^- + \text{EtCl} \longrightarrow \text{ethyl cellulose} + \text{Cl}^- \tag{4}$$

The units of Reactions (1)–(4) are moles. This means, for instance (Reaction (2)): to produce one mole of methyl cellulose one mole of CelluloseO^- and one mole of MetCl is required. The sodium ion Na^+ as well as the water in Reactions (1) and (3) and the chloride ion Cl^- in Reactions (2) and (4) are not needed to be taken into account in the modeling step.

The molar weights for the different species are given in Table 1.

Species	Molar weight
CelluloseOH	0.054 (kg/mole OH-groups)
NaOH	0.040 (kg/mole)
MetCl	0.050 (kg/mole)
EtCl	0.065 (kg/mole)

Table 1: Molar weights (kg/mole). The cellulose chain is made from glucose units, which contains three hydroxide groups per unit, see Figure 1. To simplify, the molar weight of cellulose is given in kg per mole OH-groups.

Roughly speaking, some of the hydrogen ions (H) in the hydroxyl groups in the cellulose chain (Figure 1) are removed and replaced with methyl/ethyl groups. The number of replaced groups are limited by the amounts of NaOH, CelluloseOH (or actually the number of OH-groups in the cellulose molecule) and MetCl/EtCl, according to Reactions (1)–(4). The molar weights for the removed H atom and the added groups (methyl/ethyl) are given in Table 2.

	MC	EC
Added group	0.015	0.029
Removed group	0.001	0.001

Table 2: Molar weights (kg/mole) of groups removed and added to the cellulose chain.

Summarizing the reactions, producing

$$(0.054 + 0.015 - 0.001)\text{ kg MC} \quad \text{requires} \quad \begin{cases} 0.054\text{ kg CelluloseOH} \\ 0.040\text{ kg NaOH} \\ 0.050\text{ kg MetCl} \end{cases},$$

and producing

$$(0.054 + 0.029 - 0.001)\text{ kg EC} \quad \text{requires} \quad \begin{cases} 0.054\text{ kg CelluloseOH} \\ 0.040\text{ kg NaOH} \\ 0.065\text{ kg EtCl} \end{cases}.$$

3.3 Raw material and reactors

Aditiva have four suppliers from which they buy their raw material. The suppliers are located in Lerum, Lindome, Torslanda and Vårgårda, respectively. Not all suppliers sell all types of raw materials. The prices are given in Table 3, which also shows which materials are sold by which suppliers. Aditiva buys the materials in continuous amounts.

	Lerum	Lindome	Torslanda	Vårgårda
Cellulose	100	-	-	90
NaOH	120	80	-	70
MetCl	-	-	400	380
EtCl	-	-	450	440

Table 3: Raw material costs (€/kg)

Aditiva has three different reactors that can be used for the production of cellulose ethers. These reactors are located in Mölndal, Billdal, and Gamlestaden, respectively. The costs for transporting the materials from the suppliers to the reactors are assumed to be proportional to the amount bought and are given in Table 4.

	Lerum	Lindome	Torslanda	Vårgårda
Mölndal	27.8	11.3	26.2	74.1
Billdal	44.6	12.3	30.2	91.7
Gamlestaden	19.6	19.4	21.3	59.8

Table 4: Transport costs (€/kg)

All reactors can produce both MC and EC at the same time. There are limitations on the amount of cellulose as well as on the amount of chlorides (MetCl + EtCl) that can be handled in the reactors. These limitations are given in Table 5.

Reactor	Cellulose	Chlorides
Mölndal	50	20
Billdal	30	38
Gamlestaden	15	20

Table 5: Reactor capacities – maximum amount of Cellulose and Chlorides (MetCl + EtCl) respectively that can be handled in the reactors (kg/day)

The total cost of producing, washing and purification of the ether products are reactor dependent. The costs are given in Table 6.

Reactor	MC	EC
Mölndal	50	60
Billdal	40	45
Gamlestaden	35	35

Table 6: Cost of producing, washing and purifying the cellulose ether products in the different reactors (€/kg MC (EC))

3.4 Drying

When the reactions are finished, water is let into the reactors, to wash the products and remove non-wanted bi-products. After this the reactors are emptied, and the purified products contain surplus water. Transportation to the consumers and end usage of the products demands the products to have a lower water content. For this purpose, the final products are transported to the drying equipment, located in same facility as the reactor in Mölndal. The transport cost is 6.2 €/kg MC (EC) from Billdal and 14.4 €/kg MC (EC) from Gamlestaden.

Two continuous methods of drying are used; fluidized bed and plate-style vacuum dryer, see Figures 3 and 4.

Figure 3: The fluidized bed requires that the cellulose ether must be ground to uniform particle size.

Figure 4: Ether products with different sizes can be dried in the vacuum dryer.

For optimal operation, the fluidized bed requires the products to be ground to a uniform particle size, before drying. The plate vacuum dryer is suited to a wide range of particle size distributions. Hence the two drying methods lead to two different quality classes: uniform and distributed particle size, respectively. The cost of the different drying techniques differs as well as the selling prices of the quality classes. The costs of the drying techniques are given in Table 7 and the selling prices are given in Table 8.

Method	Cost
Vacuum dryer	12
Fluidized bed, including grounding	18

Table 7: Costs of using the different drying techniques (€/kg MC(EC))

Product	Uniform particle size	Distributed particle size
MC	800	500
EC	1150	780

Table 8: Selling prices (€/kg MC(EC))

It is also possible to sell and buy non-dried MC and EC, without limitation, to a lower price. The prices are shown below. Trading of non-dried products take place in the facility in Mölndal, which means that all products produced in Billdal and Gamlestaden must be transported to Mölndal.

Product	Sell	Buy
MC	450	550
EC	550	600

Table 9: Trading prices of non-dried products (€/kg MC (EC))

3.5 The market

A thorough market analysis has been performed of the total demand of ether products with different qualities. The demand of Aditiva's products as well as the proportion of each quality is given in Table 10 below. The demand is measured on a yearly basis. It is assumed to be spread equally during the 220 days of the year when Aditiva runs production.

Product	Demand	Uniform particle size	Distributed particle size
MC	8200	60%	40%
EC	7800	45%	55%

Table 10: Total market demand on the ether products (kg/year) and the proportion of each quality

4 Assignment, Part I: Modeling

With advances in the production of plastic, plastic alternatives to cellulosic products have become increasingly competitive over time. The manufacturers of cellulosic goods, Aditiva as well, have seen their market shares shrinking recently under the pressure from substitute products and foreign producers of cellulosic goods.

Aditiva has decided to hire some consultants to optimize their production plan. If you present an easily understandable description of the problem, YOU will be chosen to perform the job and thereby earning money for your company. Now, *your task is to write a report that describes a linear programming model for minimizing the total cost, i.e., maximizing the profit, for producing cellulose ethers in Aditiva's facilities, with a time horizon of one year.* The readers of this report are your managers and also the managers of Aditiva. They are familiar neither with the problem in detail nor with optimization. Your task is to convince the managers that you should do this job!

4.1 Requirements of your report

- The model must be linear!
- The variables, parameters and constants shall be clearly defined. Be careful with the units.
- A figure illustrating the material flows of the problem shall be included and the variables illustrated in the figure.
- No pre-optimization is allowed, meaning that you cannot simplify the model in advance based on the actual parameter values. The data may change so the model should be complete.
- The report must be written with a text formatting tool (e.g. LaTeX, Word, FrameMaker).
- It shall have a professional look!!!

4.2 Tip of the day

- For the problem given in this paper it is appropriate to illustrate the flows of the different materials in a figure and then introduce a variable for each flow.
- Be careful and structure your choice of declaration of variables, constants, parameters etc. The name should be descriptive, but not too long.
- Don't be afraid to ask the assistants!
- Start in time!!!
- Use pictures!
- Read Section 8.1 in the course literature and Example 8.1 in particular.

- Since there is a lot of data in the problem, you don't need to give explicit values of the coefficients in the model; on the contrary, we encourage the use of general notation, such as d_{ij} for the cost of transporting material from supplier i to reactor j, for example. However, every coefficient introduced must be clearly defined!
- Keep the same indices throughout, e.g. let i always represent different suppliers and j different reactors.