TPA from Toluene
(recommended by Bruce Vrana, DuPont)

Terephthalic acid (TPA) is a monomer used in polyester (PET), and thus is produced in huge volumes worldwide. The normal route to TPA is the partial oxidation of p-xylene, an expensive starting material. This oxidation requires hydrogen bromide as a catalyst promoter, thus necessitating expensive materials of construction in much of the process, and causing waste handling issues.

ExxonMobil has recently applied for a patent for a process, which starts with much less expensive toluene. Toluene is reacted in an ionic liquid (aluminum chloride and methylethyl imidazole) with carbon monoxide to produce tolualdehyde, predominantly the para isomer. Tolualdehyde can then react much the same as p-xylene in the conventional oxidation to produce TPA. The advantage is that HBr promoter is not required with tolualdehyde, thus the oxidation plant will be much less expensive to build, and will be much more environmentally friendly.

Unfortunately, the ortho and meta isomers of tolualdehyde are also produced in the first step of the process. Separation of these isomers will be difficult. In fact, your company currently has people in the lab looking for alternative separation techniques. Vacuum distillation will be expensive, since the boiling points differ by only a few degrees, and the tolualdehyde must be at least 99.99% pure para isomer before going to oxidation. But you will have to include that in your design, as it is the only proven technology. Your design should identify potential alternatives that the lab should investigate, and identify the incentive (i.e., just how much will the distillation cost). You should simulate this area of the plant quite thoroughly, since it is so critical.

Your company has asked your group to determine whether this new technology should be used in a new Gulf Coast plant your company is building. Your job is to design a process and plant to produce 500 MM lb/yr of TPA from toluene, which is available on the site.

Assume a U.S. Gulf Coast location on the same site as a large chemical plant. The TPA must meet polymer grade specifications, and can be sold or transferred for $0.45/lb, according to your marketing organization. Toluene is expected to cost about $0.90/gallon over the long term, compared to p-xylene at $0.35/lb.
Your boss has said that a truly outstanding report would include designs not only for the ExxonMobil process, but also for the p-xylene TPA process, thus making the comparison of the two processes much easier. This kind of report would probably mean a promotion for you. Simply comparing the ExxonMobil process to the selling price of TPA means that you may be passed over for that next promotion.

The plant design should be as environmentally friendly as possible. Recover and recycle process materials to the maximum economic extent. Also, energy consumption should be minimized, to the extent economically justified. The plant design must also be controllable and safe to operate.

Reference:

World Patent Application 00/15594 to ExxonMobil.