Part a.





rate constant values













iniital conditions

differential equations

















ODE solver in MathCad was used to numerically solve for the concentration.

Part b

Solving for the maximum of the [B} vs. time solution, take the derivative and solve for the root.

Looking at the solution above, this should be somewhere around 30 minutes.







The time (min) at which the maximum [B] occurs is



The maximum [B] (mol/L) is



This corresponds to a percentage of B in the product of 66.4%.



Part c

Recognizing that the total number of moles of material is constant at 115 mol/L, we can plot

the % of each component vs. time.











Calculating the annual profit

as a function of reaction time













Note that the maximum profit of approx. $1 billion occurs at a reaction time (approx. 45.6 min) different than the time when the maximum level of B is achieved (approx. 33.4 min). This is due to the expense of unused reactant A at the shorter reaction time.

part d.

Calculating the % of D in the product at the reaction time when the profit is at its maximum indicates that this product does not meet the FDA regulations (max of 1.50 mol %).



Plotting %D vs. time indicates that the reaction must be stopped at an earlier time to meet FDA regulations.



Calculating when the % of D reaches 1.50%, we find that this occurs at approx. 33 min.









Running the reaction longer will result

in having a product that violates

FDA regulations.

So the time the reaction should be

stopped to meet FDA regulations

is 33.18 min.

At this time, the molar % of B is 64.9%



Hence to meet the FDA regulations, the maximum annual profit will be approximately $844.4 million dollars.



Note that the reaction time at which product that meets FDA regulations is shorter than

either the reaction times at which maximum concentration of B occurs or at which the maximum

annual profit occurs.

Clearly running the reaction longer increases the annual profit. The issue is how to meet FDA

regulations while doing this. It may be possible to lobby to change the regulation, develop a

way to remove D from the product, or inactivate/reduce the toxicity of D by chelating/absorbing

it onto an inert carrier (e.g. clay, cellulose, proteins, etc.