MINIPROJECT #1

Lactic acid esters are interesting bio-based and biodegradable green solvents fully miscible with water. The project deals with studies on equilibrium esterification of the acid by a mixture of methanol (1) and ethanol (2) according to the following scheme:

(1)
$$H_3C \rightarrow OH + H_3C-OH$$
 cat. $COH_3C \rightarrow CH_3 + H_2O$

(2) O CH₃C OH
$$+$$
 H₃C OH CH₃C $+$ H₂O

- 1. A mixture of 500g of ethanol (96 wt.%*), 500g of methanol (100 wt.%), 1000g of lactic acid (85 wt.%*) and a catalyst was stirred in a closed reactor at a certain temperature until equilibrium reached. Calculate the molar concentration of species knowing that equilibrium constants expressed in molar concentrations (mol/L) are equal to $K_1 = 11$ and $K_2 = 25$. Validate your results. *) Commercially available purity, the second component is water.
- 2. Based on developed model propose the initial composition of the mixture of lactic acid, ethanol, methanol, water (in grams*), yields equimolar (or close to equimolar as possible) amounts of methyl lactate and ethyl lactate under equilibrium ($K_1 = 11$ and $K_2 = 25$).

 *) Commercially available purity i.e. ethanol 96 wt.%, lactic acid 85 wt.%.

The project should contain Python code used for calculations along with your brief comments explaining the most important parts of the code as well as your assumptions and results you got.