CUMCM-2021 Problem B

Preparation of C4 Olefins from Ethanol

C4 olefin is widely used in the production of chemical products and pharmaceutical intermediates, and ethanol is an important raw material for production and preparation of C4 olefins. During the preparation process, the catalyst combination (i.e. the combination of Co loading, charging ratio of Co/SiO2 and HAP, ethanol concentration) and temperature will affect the selectivity of C4 olefins and the yield of C4 olefins (see appendix for the explanation of terms). Therefore, it is of great significance and value to explore the process conditions of preparing C4 olefin by the catalytic coupling of ethanol through the structure design of the catalyst combinations.

A series of experiments on different catalyst combinations under different temperatures are conducted by a chemical laboratory. The results are shown in Annex 1 and Annex 2. Please complete the following questions through mathematical modeling based on the data provided by the experimental results:

(1) For each catalyst combination in Annex 1, please explore the relationship between ethanol conversion rate, C4 olefin selectivity and temperature respectively, and analyze the experiment results of the catalyst combination given in Annex 2 at 350℃ at different times.

(2) Please explore the effects of different catalyst combinations and reaction temperatures on ethanol conversion rate and C4 olefin selectivity.

(3) How to select different catalyst combinations and reaction temperatures to make the C4 olefin yield as high as possible under the same experimental conditions? If the temperature is lower than 350℃, how to select the catalyst combination to make the yield of C4 olefins as high as possible?

(4) If 5 more experiments are added, how do you design them, and give detailed reasons for your design.

Appendix: Explanation of terms

Temperature: reaction temperature.
Selectivity: the proportion of a certain product in all products.
Time: the reaction time of the catalyst in an ethanol atmosphere (in minutes).
Co loading: the weight ratio of Co and SiO2. For example, "Co loading is 1 wt%" means that the weight ratio of Co to SiO2 is 1:100, which is recorded as "1wt% Co/SiO2".
HAP: hydroxyapatite, a catalyst carrier.
Charging ratio of Co/SiO2 and HAP: refers to the mass ratio of Co/SiO2 and HAP. For example, "A14 (33mg 1wt% Co/SiO2-67mg HAP， ethanol concentration

1.68ml/min)" means that the weight ratio of CO to SiO2 is 1%；the mass ratio of Co/SiO2 and HAP is 33mg: 67mg；and ethanol is added in 1.68ml per minute.

Ethanol conversion rate: the one-way conversion rate of ethanol per unit time，it equals

100%× (ethanol intake - ethanol residue) / ethanol intake.

C4 olefin yield rate: C4 olefin formation rate，it equals

ethanol conversion rate × C4 olefin selectivity.

Annex 1: Performance data table, where Ethylene, C4 olefin, Acetaldehyde, Carbon number 4-12 fatty alcohol, etc. are products of reaction. Loading mode I is used from labels A1~A14, and loading mode II is used from labels B1~B7 in the catalyst experiments.

Annex 2: Experiment data at 350 degrees for a given catalyst combination.