YOHIMBINE SYNTHESIS USING FED-BATCH FERMENTATION

Initially a fed batch module was created using the previously existing batch fermentation model in biosteam. Kinetic equations have been replaced by the ones corresponding to fed batch process. The modified equations which elucidate the oxygen dependency was used. The kinetic parameters, yield coefficients and other constants used in the calculation of oxygen dependency of the fermentation has been assumed. The python file including the equations and constants has been separately uploaded. The volume was fixed as given in the assignment. Feed stream was not altered from the biosteam example.

Setting the chemical was problematic since biosteam does not recognize several thermodynamic properties of yohimbine probably due to its state. If yohimbine is imported using CAS ID as given in the library, the reaction would give several errors due to the lack of enthalpies. I was unable to carry on with these typical methods. Also, it was not possible to set molecular weight of new compound either. Thermosteam has a provision to add new model using Antoine's equation. This was applied here with assumed A, B, C values. Boiling point is taken from predicted data in Chemspider. Other values are copied from ethanol for the time being.

Indole alkaloids like such as serotonin are usually biosynthesized from yeast by employing several enzymes and complicated pathways. The typical alcohol fermentation equation which exists in biosteam had to be changed. Due to the presence of nitrogen group in the product, a N-source must be added to the reactant side. Balancing the reaction with a nitrate group on the LHS proved a difficult task. Altering the fermentation reaction causes several errors due to parameters in thermosteam/reaction and hence it has not been changed.

The chosen downstream process for this assignment is a combination of liquid-liquid extraction and distillation. LLE was chosen since it is a common technique used when yohimbe is extracted after grinding the barks of yohimbe trees. Usually, alcohols are used for this process so ethanol is chosen here. From the fermentation outlet, only mixer settlers have the provision to add solvent but due to low flowrates, the vessel sizing is warned to be out of bounds.

To remove the ethanol and to concentrate the yohimbine product, a distillation is considered for the second downstream process. The working temperature and pressure should be low so that yohimbine does not undergo degradation. Ideally the solvent would be later removed by drying or crystallisation and yohimbine product can be obtained.

The system was connected between the 3 units using manual_sys and the TEA for the whole system was carried out following the documentation given in biosteam. The file _fedbatchTEA was coded and used for this and the values as well as the time range used has not been altered from the biosteam example. Cash flow table was printed as well.

The values in the results are extremely low quantities and the expected product is also found in the top product of distillation. This is probably due to the crude assumptions I have made throughout the assignment. I think result would be slightly better with real values.

References

1. *https://patents.google.com/patent/CN102863439A/en*
2. *https://www.frontiersin.org/articles/10.3389/fmicb.2018.00670/full*