## Component specification

\*Data format: excel file.

Data pretreatment: Since raw data from anaerobic process (This wastewater has the potential for producing methane.) is difficult to find, I will create excel file mimicking the data based on two references. One data is from anaerobic process for dissolved methane evaluation, and another data is from nitrogen removal reactor. Both data will first evaluate 1-month daily data, and then broaden to 1-year daily data.

The excel file for dissolved methane calculation will include water quality value: chemical oxygen demand (COD), biological oxygen demand (BOD), salinity and temperature. The excel file for nitrate consumption evaluation will include nitrate and nitrite concentration for nitrate/nitrite anaerobic methane oxidation (N-DAMO) process removing nitrogen.

## **Software component:**

Goal 1: dissolved methane calculation

- Pandas for reading excel data=pd.read\_excel (file path)
- 2. Selecting methane potential data

Columns: "COD", "BOD"

Index: Time in days

Unit of values: mg BOD or COD/L

Save data as df1

3. Methane conversion from COD and BOD.

methane=0.25\*df1

Unit of values: mL methane/L

- 4. Selecting factors influencing methane dissolved
  - a. Temperature (temperature will usually be monitored in the wastewater treatment plant)

Columns: "temperature"

Index: Time in days
Unit of values: °C

Else if function to determine different temperature influencing produced methane dissolved in water.

Save data as df2

- b. Salinity (salinity might not be included in the wastewater treatment plant)
  Else if function to write how different level of salinity influencing dissolved methane.
- c. Combine the result of temperature and salinity for dissolved methane modified

parameters.

df4=df2\*df3

5. Choosing the minimum methane for the least methane produced by the wastewater.

Else if function for choosing which methane produced by COD or BOD is smaller

Columns: "COD", "BOD" (data frame is df4)

Index: Time in days

Unit of values: mL methane/L

Goal 2: nitrate consumption based on dissolved methane

- 1. Pandas for reading excel (This is another excel file for nitrate removal evaluation.) data=pd.read excel (file path)
- 2. Selecting nitrate and nitrite for evaluation.

Columns: "nitrate", "nitrite"

Index: Time in days
Unit of values: mg-N/L

- 3. Calculate nitrate removal by dissolved methane from the result of dissolved methane calculation.
  - a. Nitrate conversion to nitrite
    Df4\*N-DAMO archaea reaction
  - b. Nitrite conversion to nitrogen
     (Df4\*N-DAMO archaea reaction + "nitrite")\*N-DAMO bacteria reaction
  - c. nitrate and nitrite subtracting to N-DAMO microorganisms reaction
- Visualization: plot the result of nitrate and nitrite residual after N-DAMO microorganisms reaction matplotlib.pyplot and plot for plotting

## **Interactions to accomplish use cases**

Goal 1: Interaction in dissolved methane calculation is that COD and/or BOD will have potential to convert to dissolved methane. The conversion ratio is that 1 g of COD can convert to 0.35 L of methane. From this relation, we can calculate the potential of methane production by simply uploading the excel file with the data of COD and/or BOD. The second step is using this methane conversion data to evaluate how much dissolved methane can be maintained in water body. Since dissolved methane is influenced by both temperature and salinity in different level, the else if function can be used for dissolved methane calculation. Finally, we have dissolved methane data produced by COD and BOD. We want to pick up smaller value of

dissolved methane produced by COD or BOD for Goal 2 evaluation. This action is to provide a conservative evaluation for nitrogen removal in Goal 2.

Goal 2: This goal is to use dissolved methane in the effluent of anaerobic process for denitrification, which is in the nitrogen removal tank. As a result, the dissolved methane data from Goal 1 will be used for evaluation. Nitrate and nitrite removal potential by N-DAMO microorganisms will be calculated by the stoichiometric equation while dissolved methane is assumed to be thoroughly used for nitrite/nitrate conversion. Nitrite/nitrate concentration is calculated after N-DAMO process, and the result of time and nitrite/nitrate concentration is visualized, which enables the civil engineers identify the concentration of nitrite/nitrate in the effluent after switching to N-DAMO process.

## Preliminary plan:

1. Complete Goal 1

Task includes:

- a. Data collection in anaerobic process
- b. Background investigation: Dissolved methane relation with salinity and temperature.
- c. 1-month data for preliminary test
- d. 1-year data test
- 2. Complete Goal 2

Task includes:

- a. Data collection in nitrogen removal process
- b. Background investigation: N-DAMO process.
- c. 1-month data for preliminary test
- d. 1-year data test