AVEVA Academic Competition

Energy Storage using Renewable Resources

1. Background

Energy production processes using renewable sources such as wind and solar energy have a small carbon footprint. However, the production rates of power from these sources fluctuate widely depending on the prevailing weather conditions. When electric power from renewable processes is fed to the grid, other energy producers, e.g., fossil fuel burning power plants, must modify their production rates in order to match the supply of power to the demand. This situation is illustrated in Figure 1.

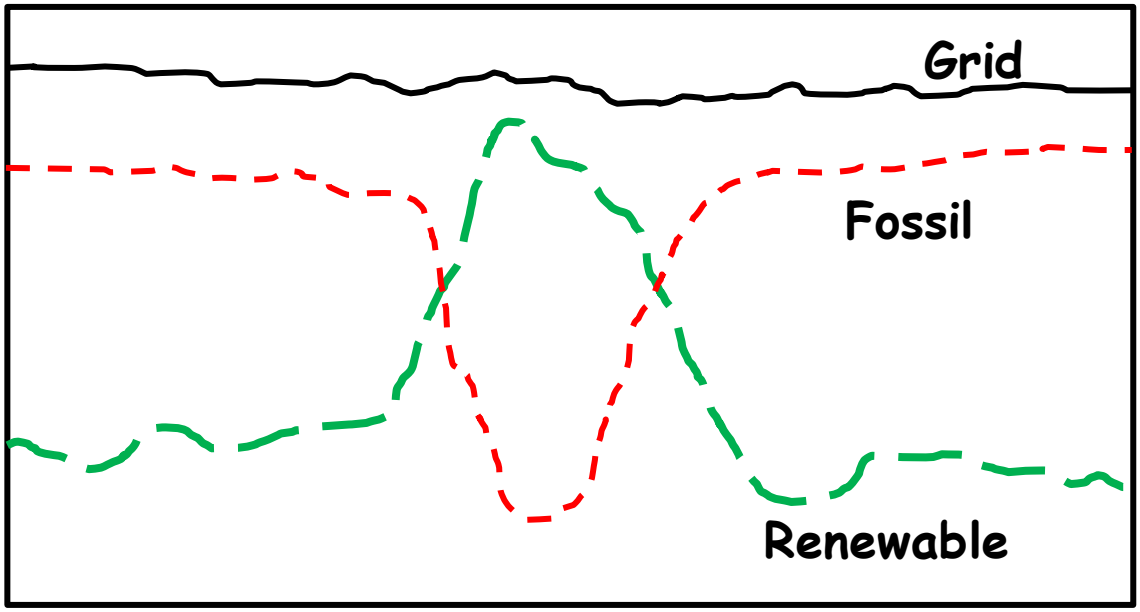

Figure 1: Typical fluctuations in renewable energy generators due to prevailing weather conditions and response of fossil fuel power generators.

The demand for electricity by users is indicated by the grid demand line in Figure 1. In general, the addition of all power from producers fed to the grid must balance the demand. The information in Figure 1 is for illustrative purposes but nevertheless shows that matching supply with demand is a continuous balancing problem. Under certain circumstances, when fossil fuel burning power plants cannot "keep up" with the fluctuating power supply from renewables, then grid stability may

be threatened and may lead to renewables being taken off-line and thus potential electric power is wasted.

The situation described previously comes about because the national grid cannot easily store significant amounts of electric energy. Currently, much research focuses on devising methods to store grid-level power/energy to overcome the problems of fluctuating renewable sources. Solutions such as large batteries, hydroelectric storage, fuel cells, and chemical storage methods have been suggested. In this project, you will look at a method to store power by converting it to a chemical building block, namely methanol.

2. Chemical Processes

In the process considered for this project, power generated from wind turbines is used to electrolytically split water into hydrogen and oxygen in a proton exchange membrane (PEM). The electrolysis plant is located close to a fermentation process, which produces ethanol. In the fermentation process, carbon dioxide is produced, and this is used as a feed stock along with the hydrogen to produce methanol. An overall block flow diagram of the process is shown in Figure 2, which is modified from the work of Matzen et al. [1].

The simulation of the transformer, hydrogen conditioning and compression, and methanol synthesis processes, shown in Figure 2, will form the basis for this project. Aveva Process Simulation (APS) version 2022, will be used for this project. It should be noted that APS has a simulation example of a solar-farm (PEM) electrolysis unit with hydrogen compression and this will be used (modified by using a wind-turbine farm) along with a new simulation of the methanol process to answer the three-part problem in the Academic Competition.

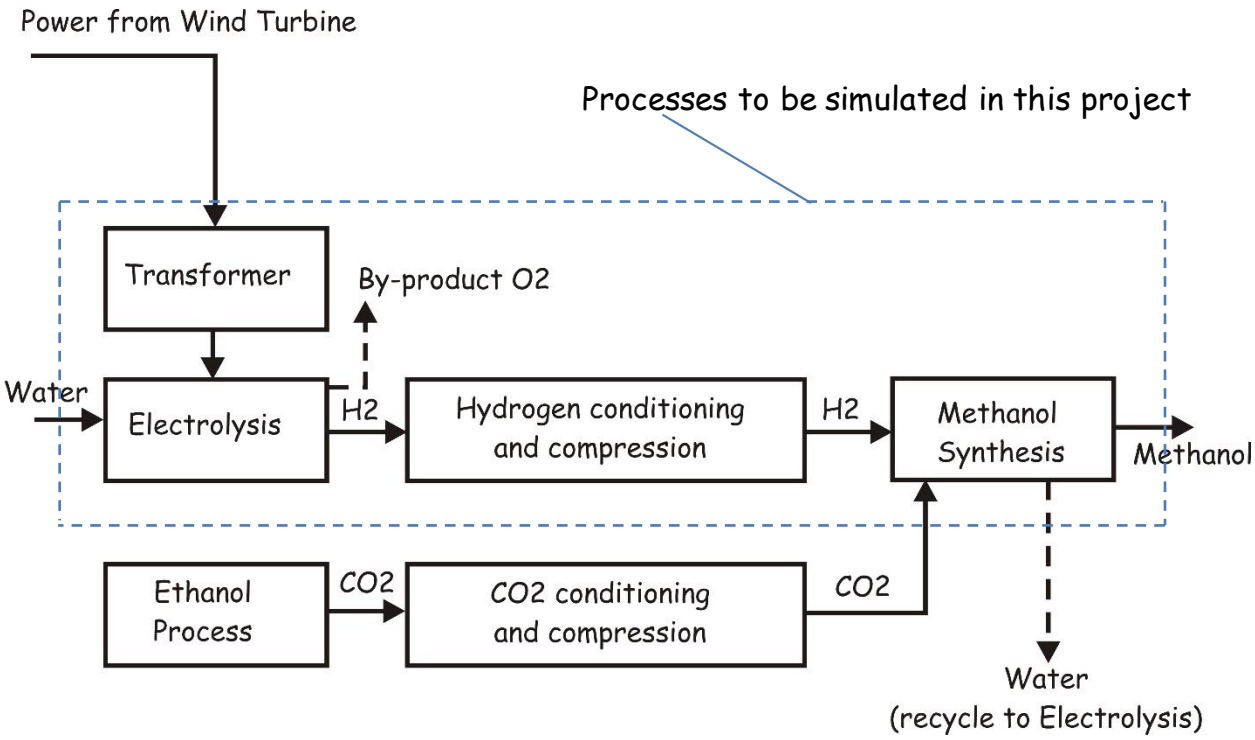

Figure 2: Block flow diagram for production of methanol using renewable power and CO_2

3. Methanol Synthesis Process

3.1 Kinetic Expressions

The production of methanol using the starting materials of hydrogen and carbon dioxide utilizes the following synthesis reactions:

$$CO + 2H_2 \leftrightarrow CH_3OH \quad (1)$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \quad (2)$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \quad (3)$$

The main reaction of interest in this work is given as Equation (2). However, because CO_2 and H_2 are present, the water gas shift reaction, Equation (3), will automatically occur and because this will result in the formation of carbon monoxide, then an additional synthesis reaction, Equation 1, will occur. The three reactions shown as Equations 1-3 are not independent and the kinetics and

equilibrium relationships can be expressed by any two of the reactions. For this problem, the kinetics of the CO and CO_2 synthesis reactions (Equations 1 and 2) will be given and the parameters are taken from the work of Song et al. [2]. Note that in the original reference, the kinetics are expressed in terms of partial fugacities, but here the kinetics are given in terms of partial pressures.

Designating the forward and reverse reactions for CO as r_{1f} and r_{1r} and the corresponding reactions for CO_2 as r_{2f} and r_{2r}, we may write:

$$r_{1f} = \frac{k_{1f} p_{CO} (p_{H2})^2}{(1 + K_{CO} p_{CO} + K_{CO2} p_{CO2} + K_{H2} p_{H2})^3}$$

$$r_{1r} = \frac{k_{1r} p_{MeOH}}{(1 + K_{CO} p_{CO} + K_{CO2} p_{CO2} + K_{H2} p_{H2})^3}$$

$$r_{2f} = \frac{k_{2f} p_{CO2} (p_{H2})^3}{(1 + K_{CO} p_{CO} + K_{CO2} p_{CO2} + K_{H2} p_{H2})^4}$$

$$r_{2r} = \frac{k_{2r} p_{MeOH} p_{H2O}}{(1 + K_{CO} p_{CO} + K_{CO2} p_{CO2} + K_{H2} p_{H2})^4}$$

Where

k_{1f} = 19.12exp(-41,770/RT)

k_{1r} = k_{1f}/K_{1eq}

k_{2f} = 639.0exp(-60,920/RT)

k_{2r} = k_{2f}/K_{2eq}

K_{CO} = 5.4913×10^{-2}exp(-246,427[1/T-1/508.9]/R)

K_{CO2} = 5.5446×10^{-4}exp(29,590/RT)

K_{H2} = 9.39343exp(-16,636/RT)

K_{1eq} = 2.2344×10^{12}exp(-118,000/RT)

K_{2eq} = 7.77×10^{8}exp(-63,500/RT)

p_i is the partial pressure of species i in MPa

r is the rate of reaction in kmol/vol of reactor/h

T is the temperature in Kelvin

R is 8.314 kJ/kmol/K

3.2 Process Flow Diagram and Description

A preliminary process flow diagram for the methanol synthesis plant is shown in Figure 3. Gaseous hydrogen (Stream 1) is fed at 890 kPa and 80°C from the PEM electrolysis unit at a rate of 775 kg/h. This is pressurized to 5,000 kPa in the feed compressor. Liquid carbon dioxide, obtained from the ethanol fermentation process (Stream 2), is fed from storage at a rate of 5766.7 kg/h as a saturated liquid at 1640 kPa and is subsequently pressurized to 5,000 kPa in the CO_2 feed pump and then vaporized in E-401. The hydrogen, vaporized CO_2, and recycled gas are combined and then fed to the reactor feed preheat exchanger, E-402, to bring the temperature to 225°C using high pressure steam as the utility. The heated stream is then fed to a shell-and-tube type reactor, R-401, that contains approximately 3300, 10 m long, 0.0762 m diameter tubes that are filled with catalyst. The reactant stream flows inside the tubes passing over the catalyst, while boiler feed water (bfw) flows in the shell of the reactor. The reactions occurring are exothermic and the bfw is vaporized to form steam at a pressure of 2550 kPa (and a temperature of 225°C). The temperature in the reactor tubes is maintained within a range of 225-240°C because of the cooling effect of the shell-side boiling process.

The reactor effluent stream is cooled in E-403 and then flashed in the high-pressure vessel (V-401) and the liquid leaving V-401 is flashed again in the low-pressure vessel (V-402). The liquid stream leaving the low-pressure flash unit is fed to stage 10 of a distillation column with 20 theoretical stages. The top liquid product is 99.9mol% methanol and the bottom product is waste water with a mole fraction of 0.0001 methanol. A vapor vent stream leaves the reflux drum and is combined with the CO_2 purge streams. In order to minimize the loss of raw materials, the fraction of Stream 7 that is recycled back to the front of the process (as Stream 8) is set as 0.99 or 99%.

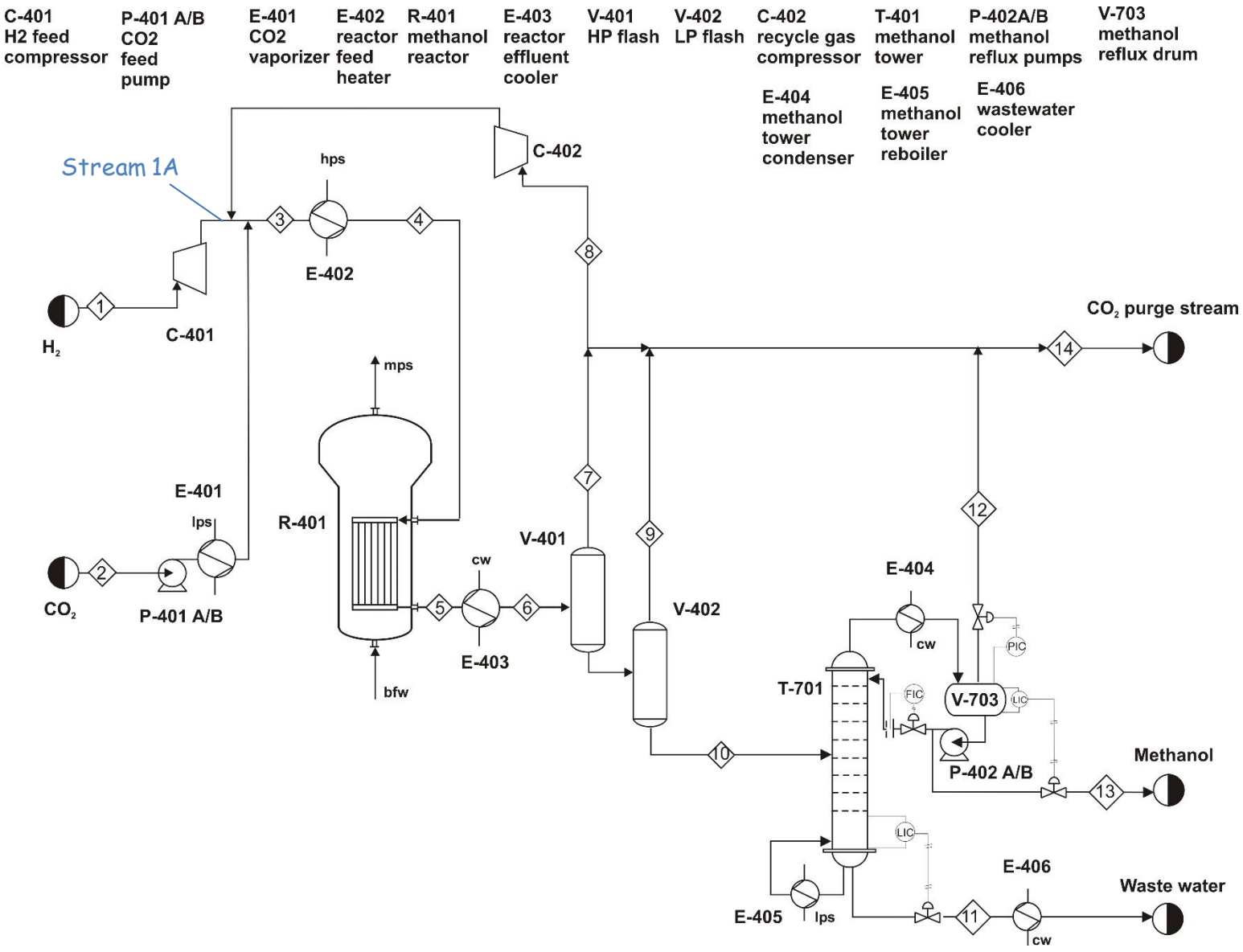

Figure 3: Preliminary PFD for Methanol Synthesis Process

4. Scope of Part 3 (available March 2, 2022, due April 1, 2022)

In the Parts 1 and 2 of this problem, you concentrated on building a base case simulation and optimizing that simulation with respect to minimizing the operating cost for the methanol synthesis process shown in Figure 3. The overall rationale behind this problem was to create a process that was "green", i.e., had a low carbon footprint and that could transform electrical energy in to chemical energy (by producing a chemical product, namely methanol). A second reason for considering this type of energy conversion process was to store electricity during times when the power produced by renewable energy sources exceeded the amount that the electrical grid could use. In this part of the project, you will consider the dynamics of the methanol process for the case when the electricity and the associated hydrogen feed rate, produced by renewable sources, fluctuates with time.

4.1 Objective of Part 3

The starting point for Part 3 of the project is given in the simulation file AVEVA_SCP_Part 3_basecase. The corresponding APS flow diagram is shown in Figure 4. This scenario is one in which the amount of hydrogen produced from the PEM units fluctuates in a sine wave around a mean value of 775 kg/h with an amplitude of approximately 75 kg/h. The fluctuation in the flowrate from this simulation is shown in Figure 5 and represents the changing feed rate to the methanol process, i.e., Stream 1 in Figure 3. Note that both Stream 1 and Stream 2 in Figure 5 are in phase and the have same amplitude (curves are superimposed). For this project, you may assume that the pressure at which hydrogen is fed to the methanol process is fixed at 890 kPa (Streams 1 in Figures 3 and 4) and that the pressure that it mixes with the recycle and CO_2 feed streams is also fixed at 4950 kPA (the pressure of Stream 1A in Figure 3 and Stream S2 in Figure 4). The fluctuations in the mass feed rate of hydrogen are generated in the dynamic simulation by using the Wave Generator (WV1 in Figure 4) and the Stream Change (SC1 in Figure 4) operations. The input boxes for each of these functional units are shown in Figure 6 for the base case. You should not change the values in the Wave

Generator input box. However, the value of the amplitude in the stream change box may have to be adjusted when solving the problem to ensure that the fluctuations in flow for stream S1 are the same as shown in Figure 5, namely, 775 ± 75 kg/h.

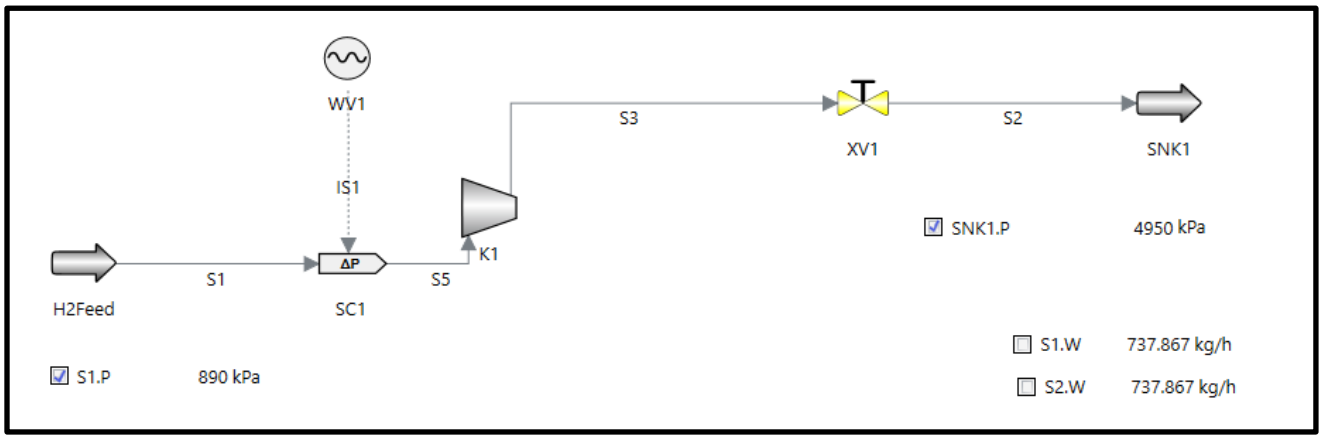

Figure 4: APS flow diagram of starting point for Part 3

(file is provided as AVEVA_SCP_Part 3_basecase)

It has been determined that fluctuations in hydrogen feed rate of ± 75 kg/h will cause the methanol process to operate in an unstable and inefficient manner. In order to ensure that the methanol process behaves efficiently , it is necessary to reduce the fluctuations in the hydrogen feed to ± 5 kg/h or smaller. Therefore, the objective of Part 3 of this problem is to change the design and implement a control scheme for the hydrogen feed section in order to maintain the flow of Stream S2 (Figure 4) to 775 ± 5 kg/h, given that the fluctuations in Stream S1 (Figure 4) vary between 775 ± 75 kg/h. You should start with the base case simulation and add equipment and controllers to fulfill this objective.

4.2 Deliverables for Part 3

The following deliverables are required for completion of Part 3.

- Submit an APS file that gives the design and control scheme needed to reduce the fluctuations in the mass flow rate of hydrogen to the methanol process to the desired level, i.e., less than or equal to ± 5kg/h.

- Submit a trend plot that clearly shows the fluctuations in Streams 1 and 2 with time. You may also want to add additional variables to this plot to help with the last deliverable.

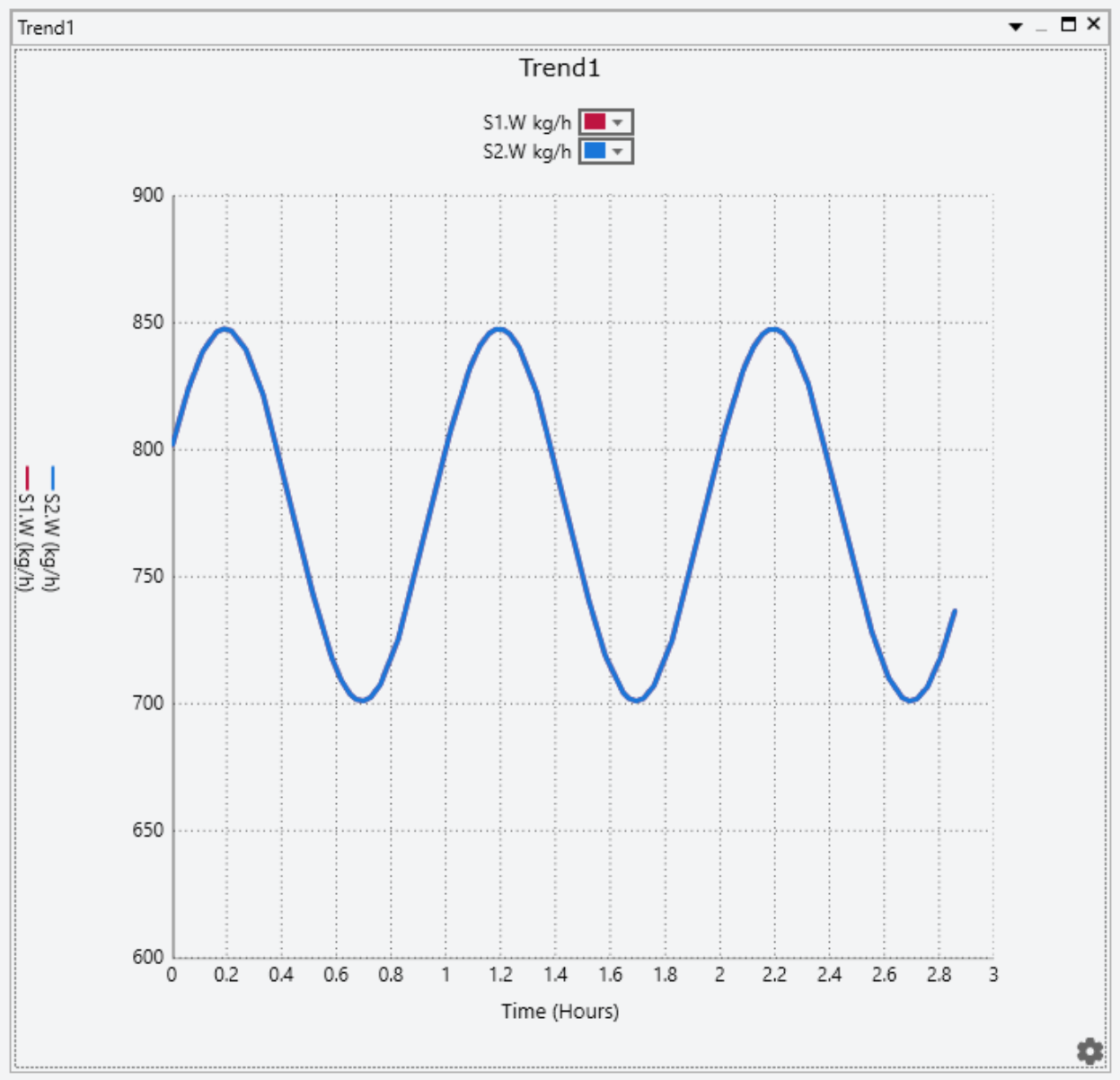

Figure 5: Flow fluctuation of pressurized hydrogen entering the methanol process as Stream 1A (see Figure 1)

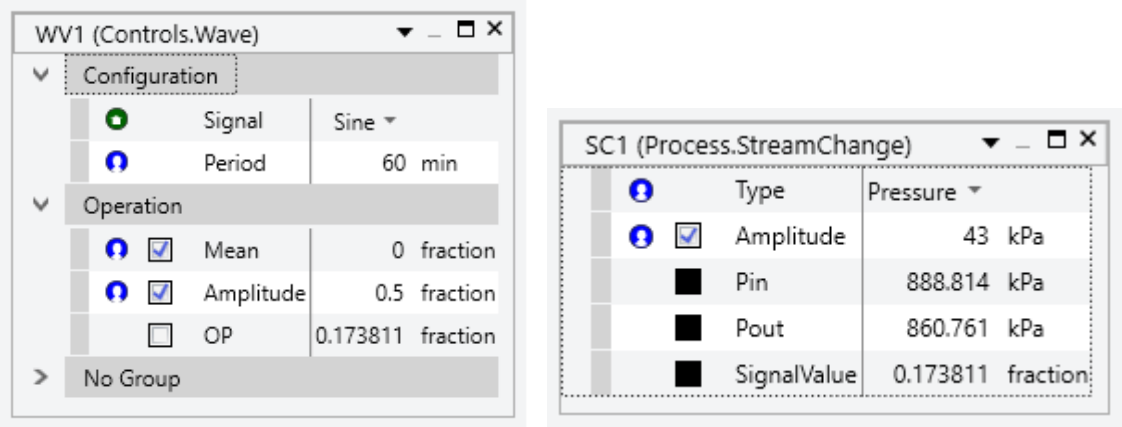

Figure 6: Wave Generator and Stream Change input screens.

- Clearly explain in 500 words or less how the control system and design changes you are recommending reduce the fluctuations in hydrogen flowrate from 775 ± 75 kg/h to 775 ± 5 kg/h.

Note: there may be several acceptable solutions to Part 3. The simpler and cheaper solutions are desired.

5. References

1. Matzen, M.J., Alhajji, M.H., and Y. Demirel, "Chemical storage of wind energy by renewable methanol production: Feasibility analysis using a multi-criteria decision matrix", *Energy* 93 (2015) pp 343-353.
2. Song, W., Zhang, J., Zhu, B., Wang, H., Fang, D., Zhu, M., and Q. Song, "Kinetics of Methanol Synthesis in the Presence of C301 Cu-Based Catalyst (I) Intrinsic ad Global Kinetics, J. Checm. Indust. Eng. (China), 4 (1989) pp 248-257