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.

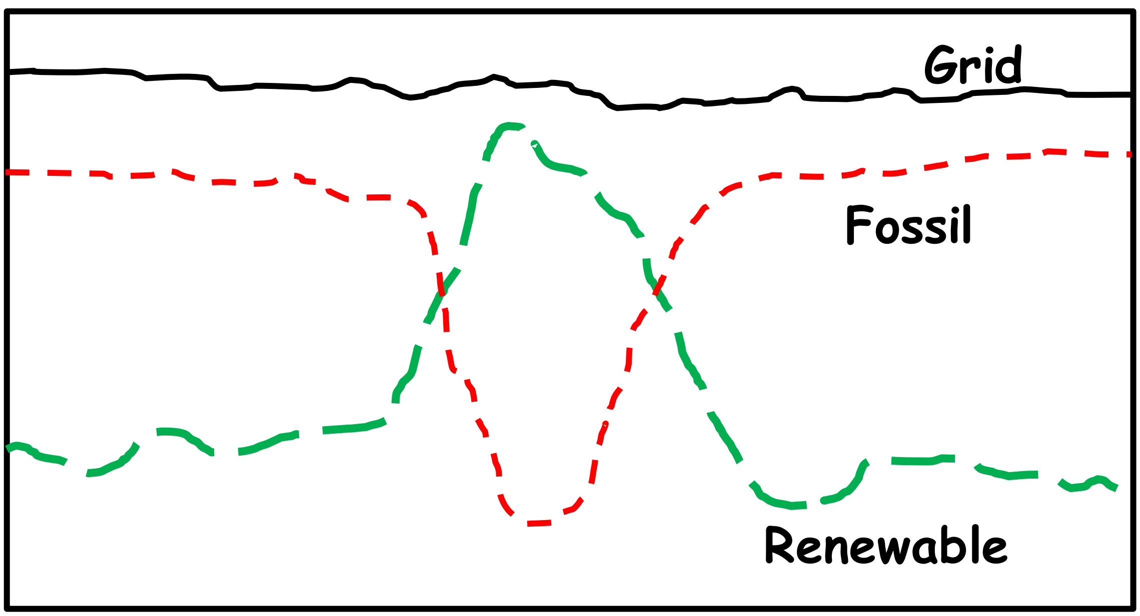

Figure 1: Typical fluctuations in renewable energy generators due to prevailing weather conditions and response of fossil fuel power generators.

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.

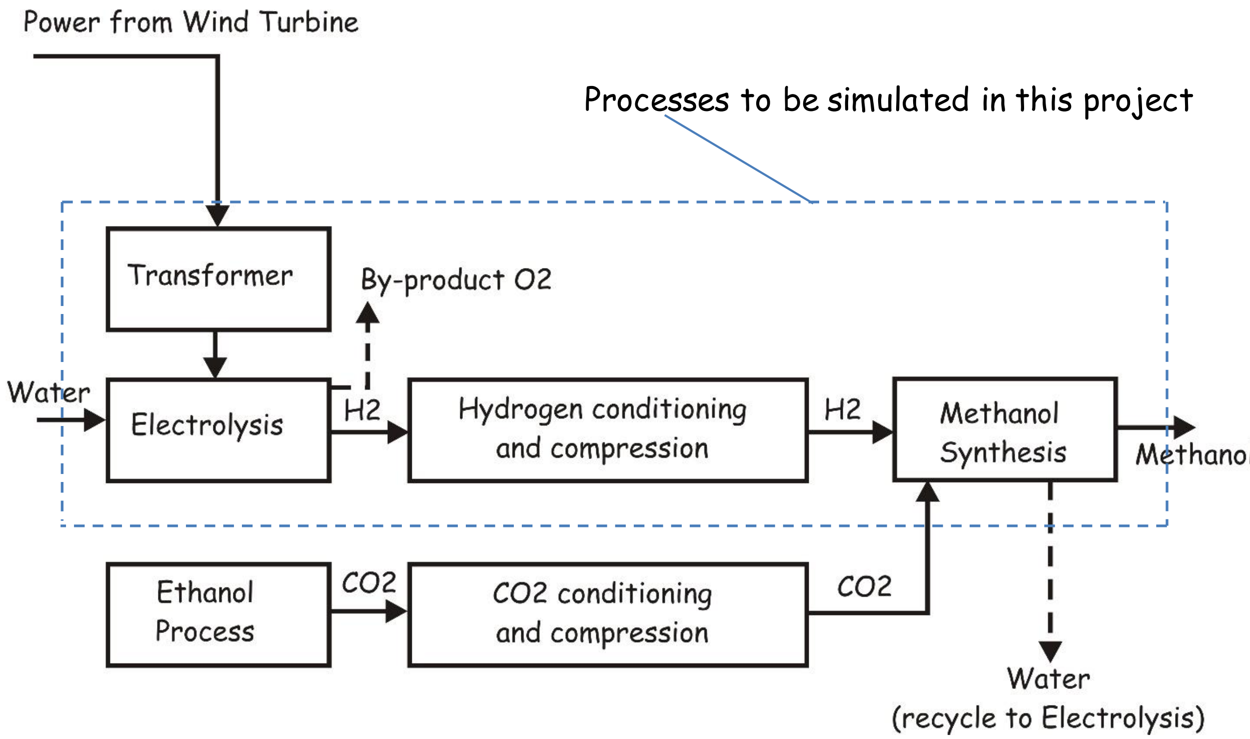

Figure 1: Block flow diagram for production of methanol using renewable power and CO_2

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:

$$CO + 2H_2 \leftrightarrow CH_3OH \tag{1}$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \tag{2}$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \tag{3}$$

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

To help you develop the kinetic model for the methanol synthesis, a file (Aveva_AC2022_MeOH_Kinetics.avi) is supplied that contains all the variables and parameters for the kinetic equations. In addition, the equations for all the reactions are included except for the reverse rate for Equation (Reaction) 2, which you will need to add to the model.

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%.

A stream table, showing flowrates, conditions, and compositions for Streams 1 -14 in Figure 3, is shown in Table 1.

4. **Scope of Design (available January 5, 2022, due February 1, 2022)**

For the first part of the student contest problem, you should perform a preliminary design of the methanol synthesis and the wind-power-to-hydrogen electrolysis processes. As stated previously, the wind-power-to-hydrogen process is given as an example file in APS and all you need to do is download this file, change the solar-farm to a wind farm, and adjust the number of wind turbines to give the desired flow rate of hydrogen, i.e., 775 kg/h. For the methanol synthesis process, you should simulate the process to give the same (or as close as possible) stream conditions (T, P, phase, and composition) as given in Table 1.

4.1 Process Hints

1. A flooding limit of 80% for tray columns should be used. Valve trays and single diameter columns are preferred. If weeping or flooding occurs in the column, then you may adjust the diameter of the column to alleviate this situation. Everywhere in the column should operate between 30 and 80% of flooding. The design for the column for this part of the project should make use of the internal condenser and reboiler options.
2. The reactor should be simulated using the "Utility" option and a heat transfer coefficient of 65 W/m^2K should be used. For the internals of the reactor, the tube length is 10 m with a diameter of 0.0762 m (3 inch). An example of a shell and tube reactor is given in the Cumene Example available in the APS package.

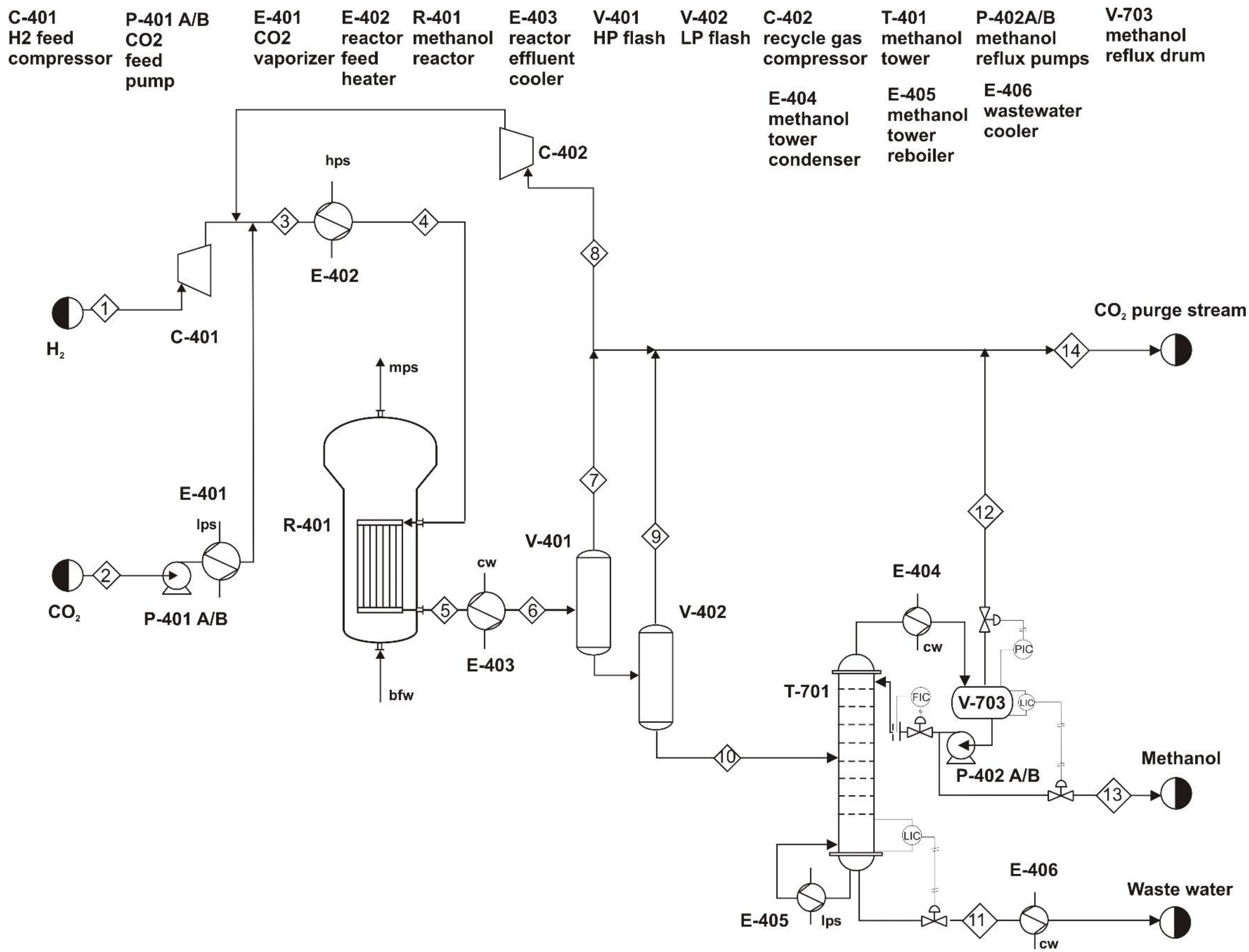

Figure 3: Preliminary PFD for Methanol Synthesis Process

Table 1: Flows for design case corresponding to the PFD in Figure 3

Stream	1	2	3	4	5	6	7
Temp, °C	80	-25.9	152.2	225.0	225.9	50.0	50.0
Pres, kPa	890	1640	4965	4950	4935	4920	4920
vf	1	1E-08	1	1	1	0.6317	1
Mass flow, kg/h	775.0	5766.7	13969.9	13969.9	13969.9	13969.9	7503.3
Mole flow, kmol/h	384.4	131.0	951.7	951.7	697.5	697.5	440.6
Comp mole fraction							
hydrogen	1.0000	0.0000	0.6893	0.6893	0.3935	0.3935	0.6226
CO_2	0.0000	1.0000	0.2863	0.2863	0.2081	0.2081	0.3242
CO	0.0000	0.0000	0.0196	0.0196	0.0271	0.0271	0.0428
methanol	0.0000	0.0000	0.0038	0.0038	0.1875	0.1875	0.0084
water	0.0000	0.0000	0.0009	0.0009	0.1838	0.1838	0.0019

Stream	8	9	10	11	12	13	14
Temp, °C	50.0	50.6	50.6	108.4	64.6	64.6	46.2
Pres, kPa	4920	200	200	133	119	119	119
vf	1	1	0	0	1	0	1
Mass flow, kg/h	7428.3	104.2	6362.5	2292.0	26.9	4043.6	206.1
Mole flow, kmol/h	436.2	2.7	254.2	127.2	0.79	126.16	7.85
Comp mole fraction							
hydrogen	0.6226	0.0447	0.0000	0.0000	0.0004	0.0000	0.3647
CO_2	0.3242	0.7637	0.0010	0.0000	0.1705	0.0009	0.4573
CO	0.0428	0.0035	0.0000	0.0000	0.0000	0.0000	0.0252
methanol	0.0084	0.1485	0.4985	0.0001	0.8291	0.9990	0.1383
water	0.0019	0.0396	0.5005	0.9999	0.0000	0.0001	0.0145

3. An operating curve for the wind turbines used in the wind farm for this project is given in the Appendix as Figure A.1. You should input this information into APS to determine the minimum number of wind turbines needed when the average wind velocity does not exceed 10 m/s .

4.2 Deliverables

The following deliverables are required for completion of Part 1.

1. A flooding profile of the methanol column showing the % flood at each tray and a statement of the diameter of the column (in m).
2. A temperature profile for the reactor and a statement of how many tubes were required,
3. A copy of Table 1 with the results of your simulation inserted.
4. The number of wind turbines and the total power required to produce the desired amount of 775 kg/h of hydrogen.
5. A converged simx file for the wind turbine electrolysis process
6. A converged simx file for the methanol synthesis process.
7. Alternatively, items 5 and 6 can be combined into one flowsheet and a single simx file can be submitted. Note that more credit will be given for Item 7 compared to Items 5 and 6.
8. A brief but informative write up, not to exceed 300 words, must be submitted that outlines how you would optimize the base case developed in this part of the problem. Note that for this assignment, you **should neither perform nor** submit any optimization work but rather you should discuss what variables you would change in order to improve the profitability of the methanol process.

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

Appendix

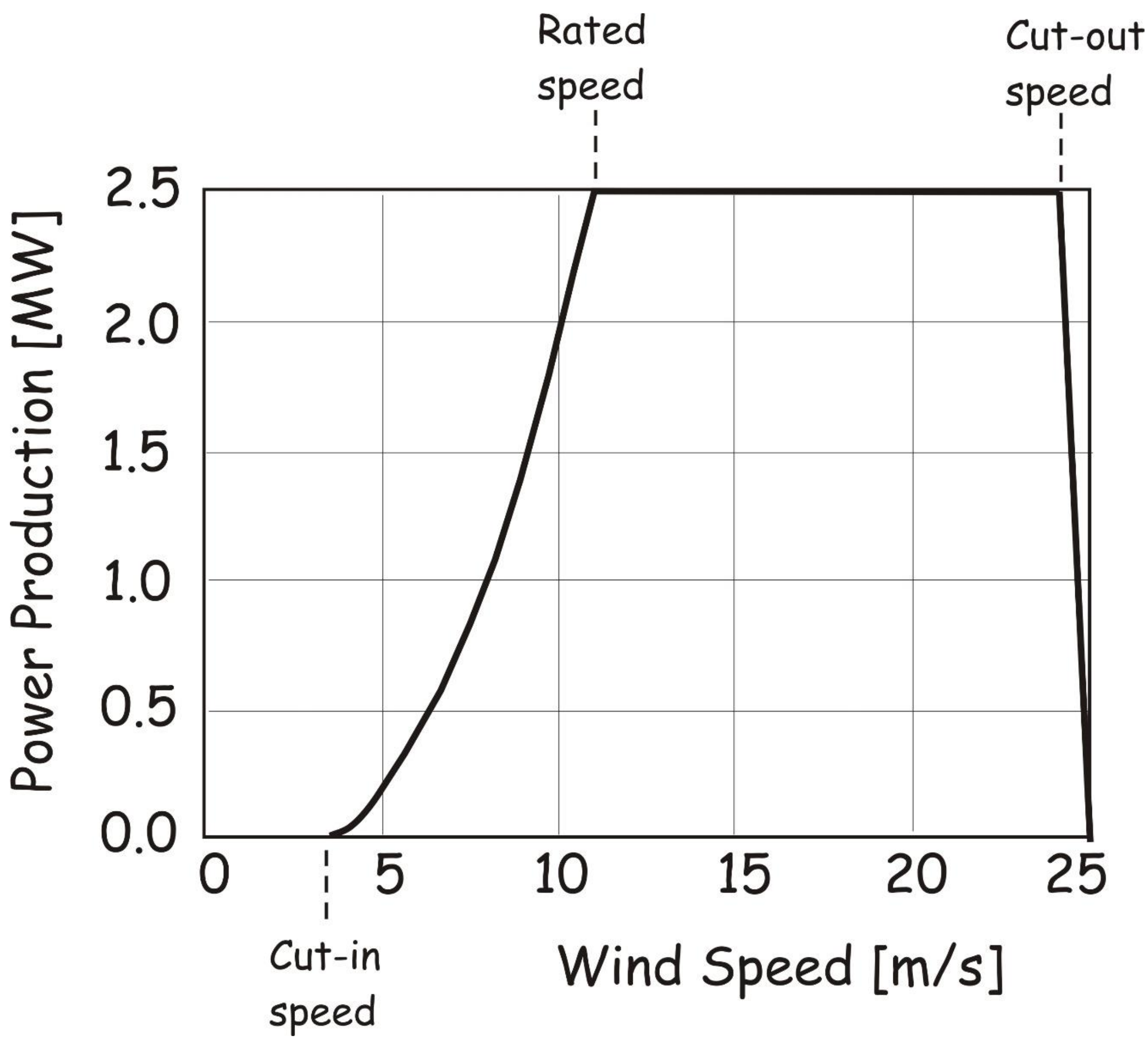

Figure A.1: Operating curve for a single wind turbine