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.

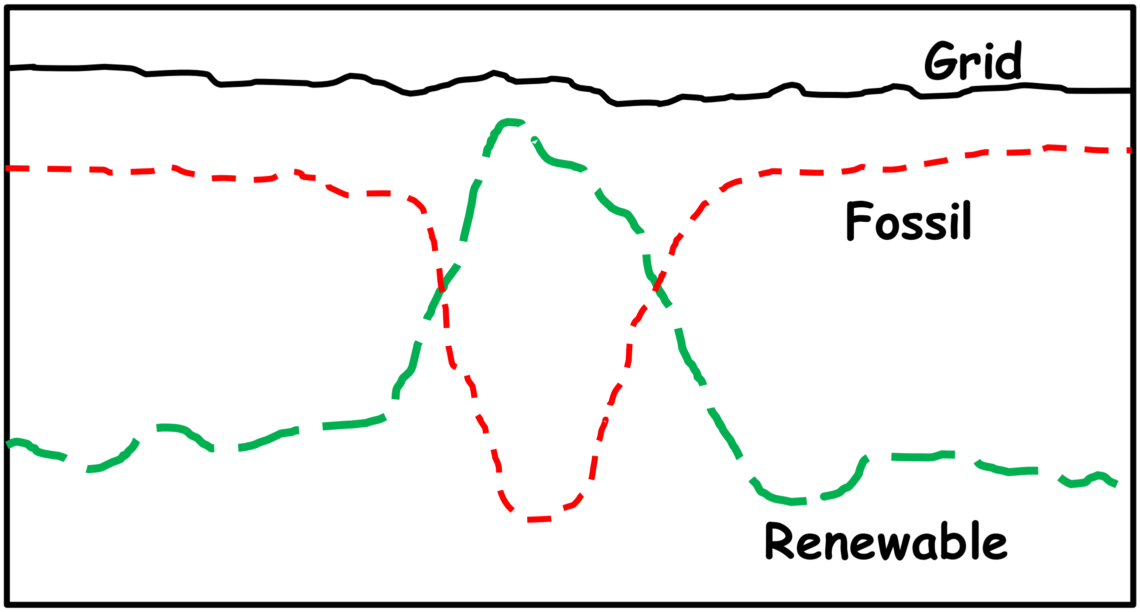

Figure 1: Typical fluctuations in renewable energy generators due to prevailing weather conditions and response of fossil fuel power generators.

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.

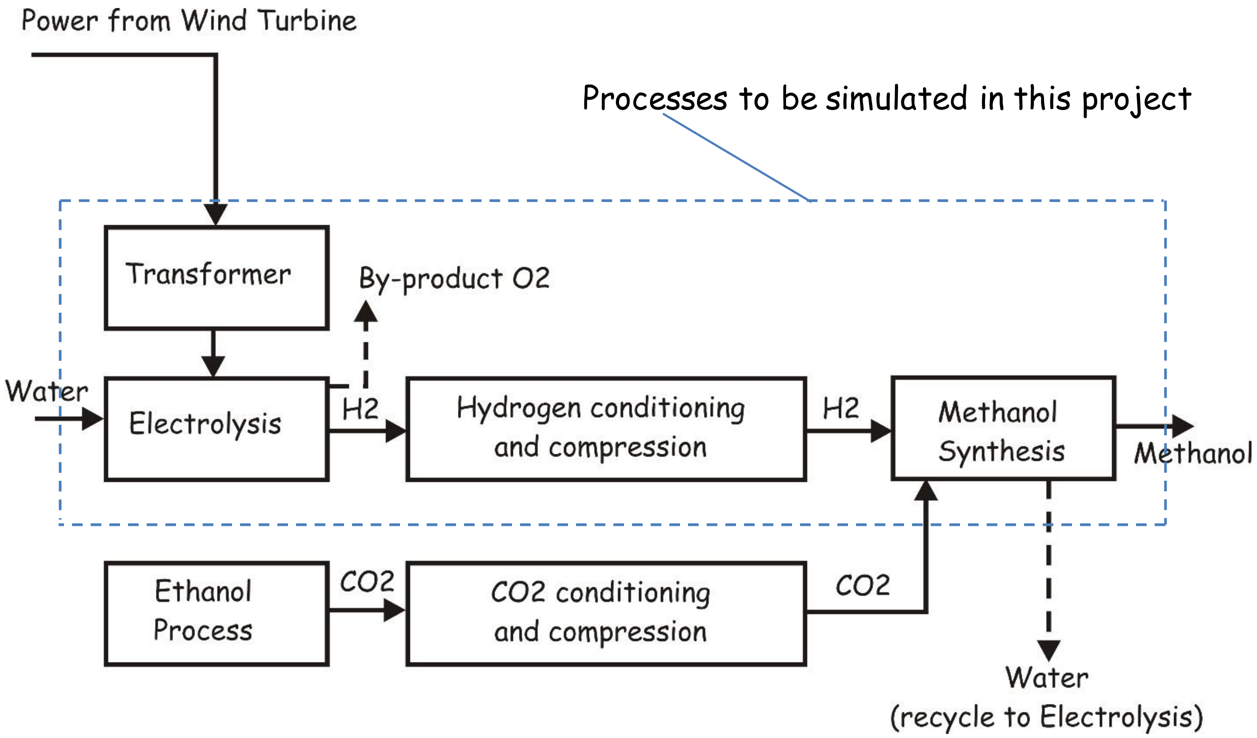

Figure 1: Block flow diagram for production of methanol using renewable power and CO_2

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:

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

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

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

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)

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

$K_{CO} = 5.4913\times10^{-2}$exp(-246,427[1/T-1/508.9]/R)

$K_{CO2} = 5.5446\times10^{-4}$exp(29,590/RT)

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

$K_{1eq} = 2.2344\times10^{12}$exp(-118,000/RT)

$K_{2eq} = 7.77\times10^{8}$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%.

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

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C-401 H2 feed compressor
P-401 A/B CO2 feed pump
E-401 CO2 vaporizer
E-402 reactor feed heater
R-401 methanol reactor
E-403 reactor effluent cooler
V-401 HP flash
V-402 LP flash
C-402 recycle gas compressor
E-404 methanol tower condenser
T-401 methanol tower
E-405 methanol tower reboiler
P-402A/B methanol reflux pumps
E-406 wastewater cooler
V-703 methanol reflux drum

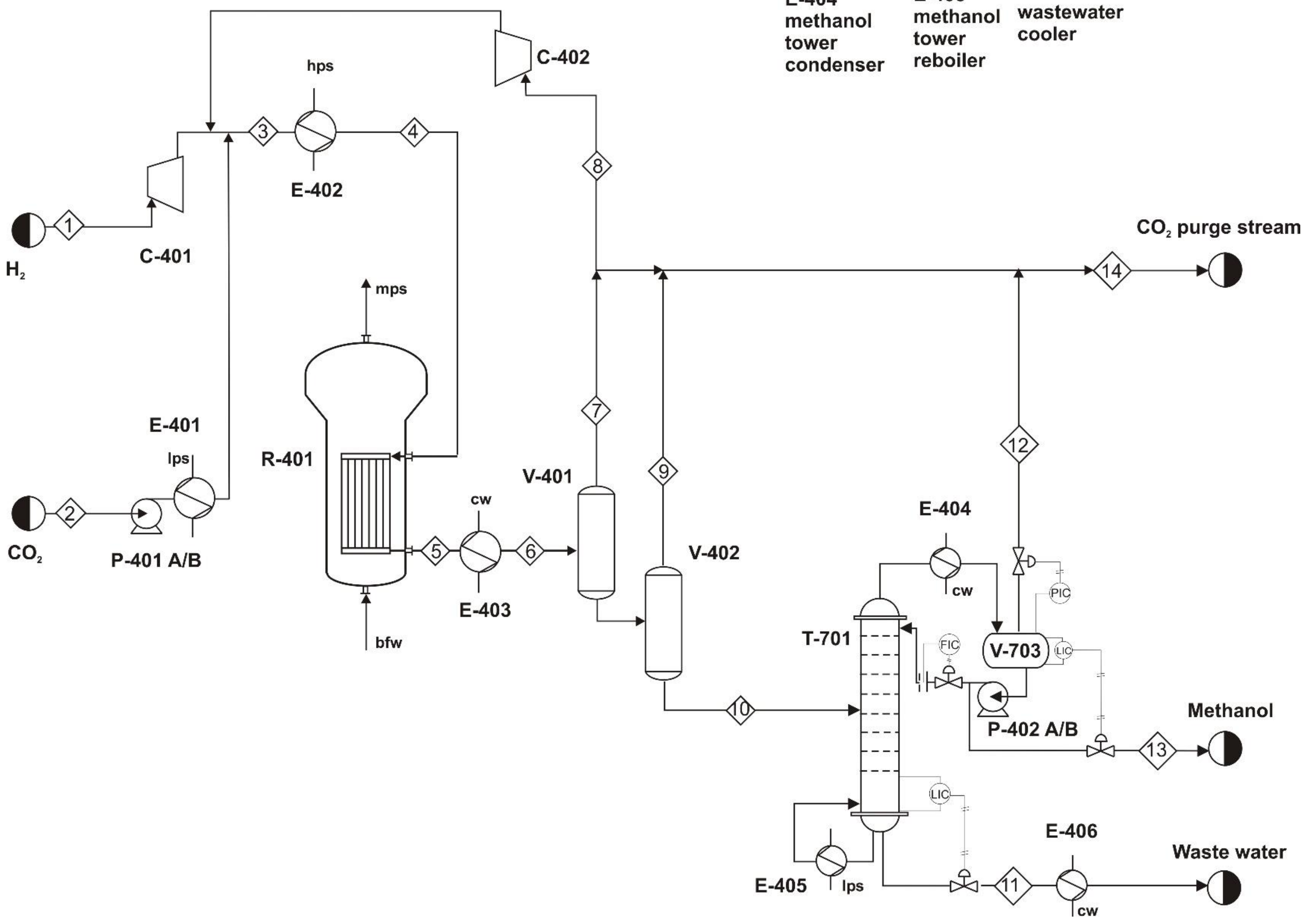

Figure 3: Preliminary PFD for Methanol Synthesis Process

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

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

In the first part of this problem, you were asked to match a base case design for the methanol synthesis process and to simulate the wind turbine farm.

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In the second part of the problem, you are asked to optimize the methanol process. To ensure a consistent starting point for all submissions, you are provided with the base case simulation corresponding to Figure 3 and Table 1. This simulation is supplied as AVEVA_SCP_Part_1.simx.

4.1 Optimization

The optimization of the process will focus on minimizing the operating cost of the process with certain constraints on the equipment. Rather than cost every piece of equipment, the following constraints are placed on the design:

a. The separation column for the methanol should not exceed 50 theoretical trays and should stay within the bounds of 30-80% of flooding using valve trays. The internal condenser and reboiler options should be used and the same product purity, i.e., 99.9mol% methanol should be maintained.
b. The size of the reactor should not exceed twice the volume (twice the number of tubes) as in the base case design.
c. The flow rates of the feeds, hydrogen and CO_2, as given in the base case are to be used and cannot be changed.
d. The minimum approach temperature in any process heat exchanger should not be less than 5°C.

With these constraints, the operating cost for the plant should be evaluated and minimized. The costs to be included in this evaluation are all utility costs, all product credits, and all utility credits. The following costs and conditions are to be used in your optimization:

cooling water (cw) is available at 300 kPa and 30°C to be returned at 40°C.
boiler feed water (bfw) is available at 110°C and 150 kPa.
low-pressure steam is available as a saturated vapor at 160°C.
medium-pressure steam is available as a saturated vapor at 200°C.
high-pressure steam is available as a saturated vapor at 260°C.
electricity is available to run pumps and compressors
refrigerated water (rw) is available at 5°C and 300 kPa and must be returned at 15°C.

The costs to be used for each of these utilities are the default values found in the APS economics tool. Note that APS uses the universal currency symbol (¤) and for this problem is equivalent to US dollars ($).

In addition, you may take a credit of $0.004/kg for any condensate from heat exchangers and any steam produced and exported from the process can be credited at a rate of $0.025/kg. The value of methanol should be taken as $1.00/kg.

It should be noted that any steam generated in a process heater must be at one of the pressures available in the plant (see conditions for lps, mps, and hps). Moreover, if steam is generated within a process heat exchanger, then boiler feed water at the appropriate pressure (via a pump) must be fed to the exchanger and paid for.

In addition to the economic optimization, you should consider the environmental impact of your design. For this purpose, use the greenhouse gas (GHG) tool in the economics tab to estimate the greenhouse gas emissions (CO_2) for the base case and your optimized process. Note that you should assume that the electricity used in the process comes from a "green" source and that the only contributor (the major contributor) to GHG is from use of steam utilities (lps, mps, and hps) imported into and used within the process. For these calculations assume that natural gas is the fuel source and use a boiler efficiency of 80% or 0.80.

4.2 Deliverables for Part 2

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) and the number of theoretical trays.
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 optimized simulation inserted.
4. A converged simx file for the methanol synthesis process.

5. Two economic summaries (using the "EconSummary" feature in APS). The first is for the base case provided and the second is for your optimized case.
6. Two GHG emissions summaries (using the "SummaryGHG" feature in APS) one for the base case and one for the optimized case.
7. A brief but informative write up, not to exceed 300 words, that describes all the changes you made to the base case design and the economic and GHG impact of each of these changes.

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

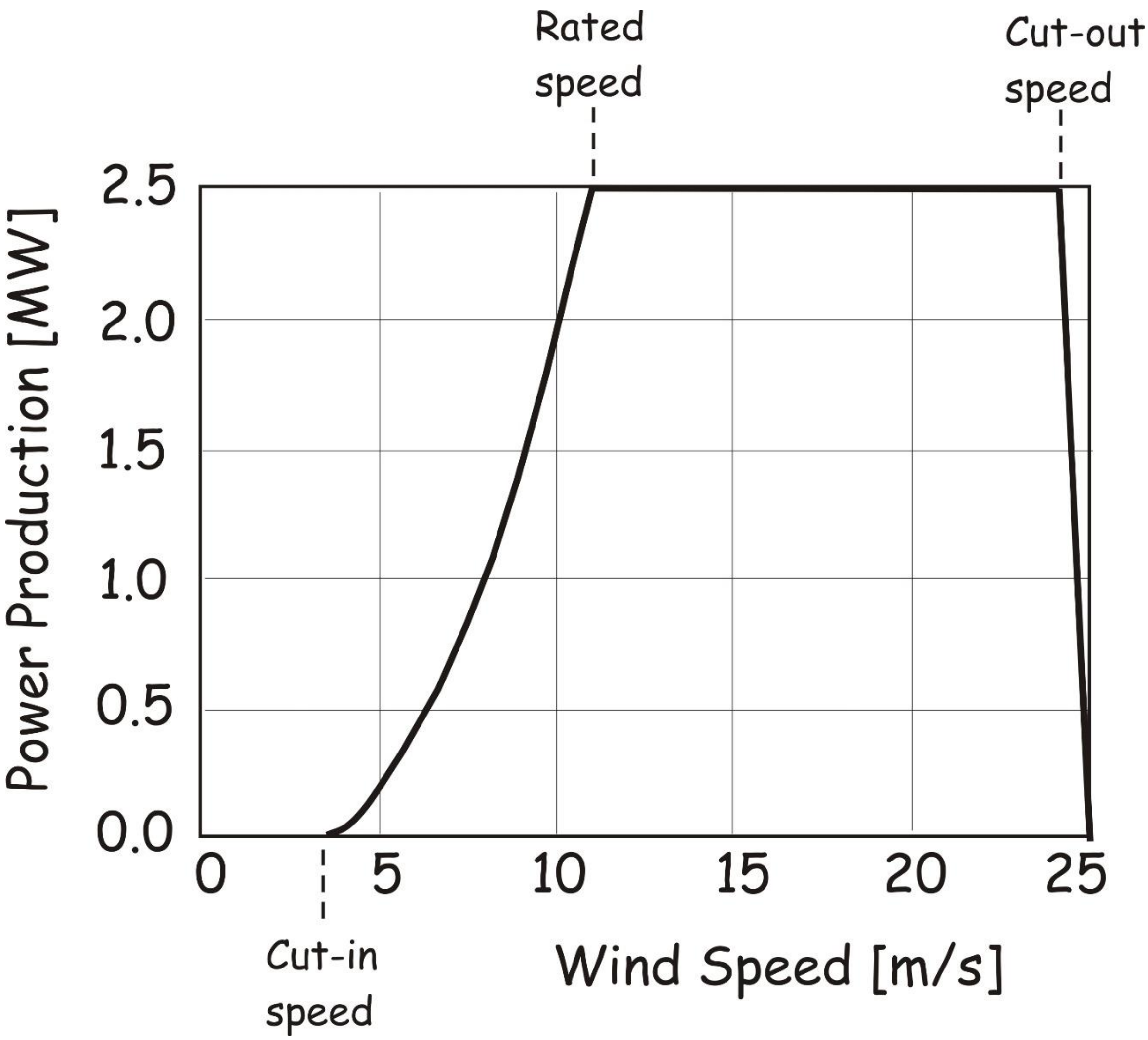

Figure A.1: Operating curve for a single wind turbine – used in Part 1