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DECO2—An Open-Source Energy System Decarbonisation Planning Software including Negative Emissions Technologies

Purusothmn Nair S. Bhasker Nair [1], Raymond R. Tan [2], Dominic C. Y. Foo [1], Disni Gamaralalage [3] and Michael Short [4,*]

1 Department Chemical and Environmental Engineering/Centre of Excellence for Green Technologies, University of Nottingham Malaysia, Broga Road, Semenyih 43500, Selangor, Malaysia
2 Department of Chemical Engineering, De La Salle University, 2401 Taft Avenue, Manila 0922, Philippines
3 Presidential Endowed Chair for "Platinum Society", The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
4 Department of Chemical and Process Engineering, University of Surrey, Guildford, Surrey GU2 7XH, UK
* Correspondence: m.short@surrey.ac.uk

Abstract: The deployment of CO_2 capture and storage (CCS) and negative emissions technologies (NETs) are crucial to meeting the net-zero emissions target by the year 2050, as emphasised by the Glasgow Climate Pact. Over the years, several energy planning models have been developed to address the temporal aspects of carbon management. However, limited works have incorporated CCS and NETs for bottom-up energy planning at the individual plant scale, which is considered in this work. The novel formulation is implemented in an open-source energy system software that has been developed in this work for optimal decarbonisation planning. The DECarbonation Options Optimisation (*DECO2*) software considers multiperiod energy planning with a superstructural model and was developed in Python with an integrated user interface in Microsoft Excel. The software application is demonstrated with two scenarios that differ in terms of the availabilities of mitigation technologies. For the more conservative Scenario 1, in which CCS is only available in later years, and other NETs are assumed not to be available, all coal plants were replaced with biomass. Meanwhile, only 38% of natural gas plants are CCS retrofitted. The remaining natural gas plants are replaced with biogas. For the more aggressive Scenario 2, which includes all mitigation technologies, once again, all coal plants undergo fuel substitution. However, close to half of the natural gas plants are CCS retrofitted. The results demonstrated the potential of fuel substitutions for low-carbon alternatives in existing coal and natural gas power plants. Additionally, once NETs are mature and are available for commercial deployment, their deployment is crucial in aiding CO_2 removal in minimal investment costs scenarios. However, the results indicate that the deployment of energy-producing NETs (EP-NETs), e.g., biochar and biomass with CCS, are far more beneficial in CO_2 removal versus energy-consuming NETs (EC-NETs), e.g., enhanced weathering. The newly developed open-source software demonstrates the importance of determining the optimal deployment of mitigation technologies in meeting climate change targets for each period, as well as driving the achievement of net-zero emissions by mid-century.

Keywords: multiperiod energy planning; negative emissions technologies; process integration; carbon-constrained energy planning; open-source software

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1. Introduction

The 17 Sustainable Development Goals (SDGs) of the United Nations are often interlinked. For example, the reduction in global poverty should be aligned with the enhancement of the health, education, and economic sectors [1]. Goal 13 is related to climate actions, which demands urgent actions to mitigate climate change impacts [1]. In 2015, 196 countries adopted the Paris Agreement aimed to limit global warming to within 2 °C and preferably 1.5 °C above pre-industrial levels [2]. Despite this agreement, countries have shown limited signs of reducing greenhouse gas (GHG) emissions. As of 2020, the average surface temperature of Earth was 1.2 °C higher in comparison to the pre-industrial period, and the CO_2 concentration in the atmosphere exceeded 410 ppm; emissions will continue to rise unless drastic mitigation actions are taken [3]. The fall in CO_2 emissions during the COVID-19 pandemic was only short-lived, rebounding to the normal trend by the year's end [3]. A shift in the economy towards carbon neutrality must occur to prevent a further rise in GHG emissions [3]. According to the IPCC [4], carbon neutrality can only be realistically achieved with the use of negative emissions technologies (NETs) in addition to other climate change mitigation measures. Any delay in mitigation actions would only compound the adverse impacts of climate change.

The need for deep decarbonisation necessitates efficient energy planning modelling tools. In response, this work develops an open-source energy system software that can be used for optimal decarbonisation planning. The mathematical formulation in this work was inspired by carbon emissions pinch analysis (CEPA) that was developed to determine the minimum deployment of renewable energy sources in meeting the CO_2 emissions limit of a geographical region [5]. Later versions of CEPA incorporated CO_2 capture and storage (CCS) [6]. However, these earlier works were limited by being unable to consider time factors, which is an important dimension in progressive decarbonisation. Energy planning models should be able to handle the temporal aspects of carbon management, involving variations in demand and CO_2 emission limits. A multiperiod energy planning model [7] was developed with the use of a CEPA-based programming framework known as the automated targeting method [8]. In comparison to the graphical technique, mathematical programming approaches are often preferable in the development of energy planning models due to their ability in handling large-scale problems. Earlier work on the superstructural model was reported as an alternative approach to solving energy planning problems similar to those of CEPA methods [9]. Later, a fuzzy integer programming model was formulated to account for the environmental and economic constraints during CCS deployment [10]. The optimal matching of CO_2 sources to available sinks was then done via a continuous-time mixed-integer non-linear programming (MINLP) model [11]. In this work, the MINLP model was simplified to a mixed-integer linear programming (MILP) model by assuming a fixed flow rate of a CO_2 source with no constraints imposed on the CO_2 storage capacities [11]. The practicality of this work was later enhanced by considering varying CO_2 flow rates and the existence of a limit on the CO_2 storage capacities [12]. The work was also made up of a multiperiod model for realistic energy planning involving CCS deployment. Following this, a further extension to the multiperiod MILP model was accomplished by considering unequal time intervals [13].

Despite these measures, the use of CO_2 removal (CDR) via NETs will still be needed for limiting global warming [4]. CDR may occur via two types of NETs, i.e., energy-producing NETs (EP-NETs) and energy-consuming NETs (EC-NETs). The former generates energy during CO_2 load removal. Some examples of EP-NETs are bioenergy with CCS (BECCS) and biochar [14]. By contrast, there is an energy penalty associated with CO_2 load removal for the latter technology. Direct air capture (DAC) [14], enhanced weathering [15] and ocean liming [16] are some examples of EC-NETs. In the past, mathematical programming and pinch-based approaches were developed to consider the deployment of NETs during carbon-constrained energy planning. For the latter approach, the graphical targeting technique [6] was extended to incorporate EP-NETs during energy planning [17]. Recognising that a portfolio of NETs would be required to accelerate CDR, this work was later revamped for the combined deployment of both EP-NETs and EC-NETs [18]. The limitations of the graphical targeting technique were overcome with the development of an algebraic targeting technique in which renewable energy sources, CCS and NETs were considered during energy planning [19]. An optimal source-sink matching for CDR via biochar was initially conducted via a MILP model [20]. The objective function of the model was set for the maximisation of CDR without compromising the soil quality [20]. Other work involving biochar was performed via a fuzzy linear programming model involving biomass co-firing in power plants [21]. Aside from biochar, EW is also an effective means of CDR, with several mathematical programming approaches being developed previously to account for its deployment [15]. The optimisation of EW networks initially took place via a linear programming (LP) model [22]. Due to the uncertainties with EW networks in terms of silicate rock grinding and property variations, a fuzzy MINLP model was formulated to address these issues [23]. The fuzzy model was further enhanced to consider the uncertainties that exist within industrial supply chains and economic evaluations [24]. A recent work considered the use of non-hazardous industrial waste during EW, in which a superstructural model was developed for its evaluation and analysis [25]. Since large-scale CDR would require a portfolio of NETs, an LP model was formulated to optimise NETs' deployment under resource (e.g., land, water, nutrients, and energy) constraints [26]. Due to a projected extensive deployment of EW, a stand-alone supply chain-like system would exist, thus presenting a need for its optimisation. Therefore, a more recent work aimed to use a MILP model for the optimisation of the processes that occur in an EW network [27].

Given the urgent need for decarbonisation, energy planning tools have been developed to aid in policymaking and the planning for future energy generation. The two major energy planning modelling tools that are typically employed are the bottom-up and top-down models. The former model is focused on the components of an energy planning system, i.e., the availability of various technologies, and the overall costs involved [28]. In other words, the target demand and emission limits are satisfied based on the technologies made available in a period and the allocated budget [28]. Meanwhile, the latter model investigates the impact of set demand and emissions limit targets on the economic and energy sectors [29]. In other words, the top-down model investigates economic impacts due to the implementation of such energy policies. In this work, a novel bottom-up model is developed due to the availability of a wide technology library, aside from cost constraints. Therefore, the discussion of existing energy planning models will be tailored to those that have employed the bottom-up model.

An example of a bottom-up energy planning model is the Wien Automated System Planning model [30]. A user can add energy planning constraints such as fuel availabilities, system reliability targets, and emissions limits [30]. The model then determines the optimal configurations for the expansion of existing energy systems by considering the costs involved in existing and new plants [30]. Another integrated energy planning model is OSeMOSYS [31]. Aside from providing detailed power configurations, this energy planning model also considers multi-resource (i.e., economic, material and energy) systems [31]. More recently, OSeMOSYS integrated smart grids to deal with intermittent renewable energy sources [32]. One of the most popular energy planning models is MARKAL [33]. This energy planning model consists of a pool of technologies with their associated costs and emissions constraints. Based on the demand of the energy planning system, a range of technologies that minimise the total costs was selected [33]. TIMES is another energy planning model, which is an extension of MARKAL that integrates an economic approach to supplement the existing technical approach [34]. The solutions obtained from TIMES are based on scenario analysis. A base case is developed as a reference for the addition of interventions (e.g., minimum deployment of renewable energy, permissible emissions limits, etc.). Once the constraints are incorporated, a separate scenario is then developed and compared against the base case, which then allows the users to select the best possible scenario after the evaluation of multiple scenarios [34]. Table 1 presents a summary of the existing bottom-up energy planning models available for deployment.

From Table 1, it can be observed that in all existing energy planning models, little focus has been placed on the key role that NETs and CCS can play in the future. Note, however, that both of these technologies must be incorporated to align with the targets set during the Paris Agreement [2] and the Glasgow Climate Pact [35]. Therefore, this work reports the development of a Decarbonisation Options Optimisation (*DECO2*) software tool that consists of a pool of technologies, including CCS and NETs, that may be employed to meet the CO_2 emissions limits at specific facilities, along with new generation capabilities and decommissioning strategies. There has been no such work conducted in the past that includes all types of mitigation technologies (i.e., renewable energy, CCS and NETs). Additionally, previous works did not consider the commissioning and decommissioning timeline of power plants. This aspect must be considered for realistic energy planning of deep decarbonisation. The multiperiod energy planning model in this software may be employed by policymakers to determine long-term decarbonisation strategies. The latter includes the timeline for the decommissioning of plants, technology implementation, and fuel substitutions for fossil-based power plants (to renewable energy sources). The mathematical programming in the software is expected to provide rigorous optimal solutions, subject to constraints such as the availability of low-carbon fuels and renewable energy sources, technology readiness, etc. The paper is organised as follows. A formal problem statement is presented in the next section. This is then followed by the mathematical formulations for carbon-constrained energy planning. The software infrastructure is then presented to demonstrate the software application. Two scenarios of a hypothetical case study that differ in terms of the deployment of mitigation strategies are presented to show the applicability of the *DECO2* software. Finally, conclusions and prospects for future work are provided.

Table 1. Summary of bottom-up energy planning models.

Energy Planning Models	Features	Missing Key Feature
WASP	- Power generation systems - Fuel availabilities and emissions limits - Optimal expansion of existing energy systems - Cost of existing and new energy generation plants	CCS and NETs for individual plants
OSeMOSYS	- Integrated assessment for energy planning - Multi-resource systems (economic, material and energy)	
MARKAL	- A pool of technologies for satisfying emissions and cost constraints	- NETs' deployment - Open-source software - Commissioning and decommissioning strategies - Technology implementation time - Easy-to-use input spreadsheet
TIMES	- Extension to MARKAL - Incorporates economic approach - Viewing multiple energy planning scenarios	

2. Problem Statement

The formal problem statement for the development of a process integration-based software tool for optimal decarbonisation is as follows:

- A pool of fossil-based (coal and natural gas) and renewable energy-based (solar, hydropower, etc.) plants are available to satisfy the energy demand and CO_2 emissions limit of an energy planning system in period $k \in K$.
- Power plant i has a lower-bound energy output ($F_{i,LB}$), an upper-bound energy output ($F_{i,UB}$) and CO_2 emissions intensity (CS_i) that make up the energy planning system for period $k \in K$.
- The commission and decommissioning periods for power plant i are specified.
- The total energy demand (D_k) and CO_2 emission limit (L_k) of the energy planning system in period $k \in K$ are specified.
- The removal of the CO_2 emissions in period $k \in K$ is aided by the deployment of renewable energy source $r \in R$, CCS technology $n \in N$, EP-NETs technology $p \in P$, EC-NETs technology $q \in Q$, alternative solid-based fuel $s \in S$ and alternative gas-based fuel $g \in G$.
- The main task is to determine the energy generation from power plant i and the minimum deployment of each technology (renewable energy, CCS, NETs and alternative fuel) in satisfying the demand and CO_2 emissions constraints of an energy planning system in period $k \in K$.

Figure 1 presents a superstructure representation of the process integration-based software for optimal decarbonisation.

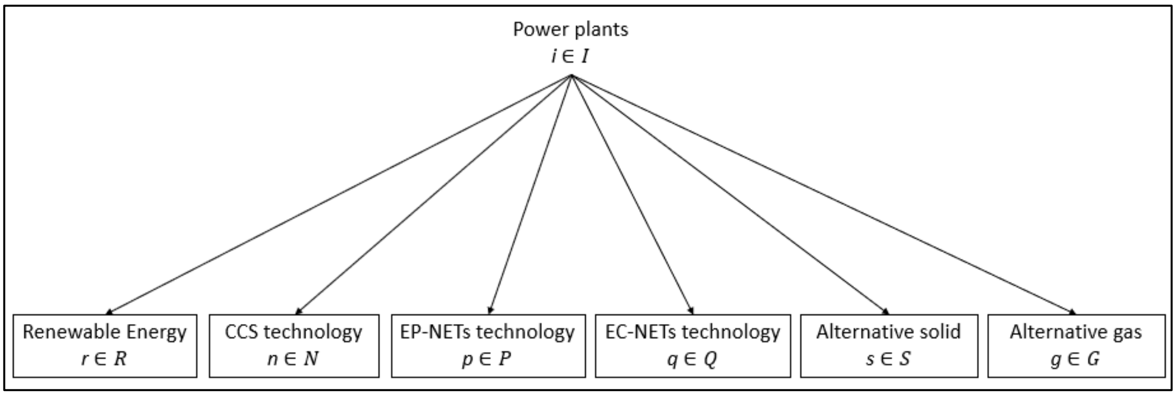

Figure 1. Superstructure representation of the process integration-based software for optimal decarbonisation.

3. Mathematical Formulation of *DECO2*

DECO2 is based on a superstructural model, consisting of existing and upcoming power plants available for power generation, as well as a pool of mitigation technologies. The superstructural model initially determines the energy generation from power plant i that satisfies the power demand of energy planning period k. Following this, the optimal deployment of mitigation technologies, i.e., renewable energy sources, CCS, NETs and alternative fuels, in period k is determined based on the demand and CO_2 emissions constraints. The superstructural model developed in this work would act as a guide to policymakers in terms of power plants' commissioning and decommissioning timelines and total costs involved in meeting the energy demand and CO_2 emissions limits of a geographical region.

First, the cumulative deployment of energy source from power plant $i \varepsilon I$ should satisfy the energy demand of period k, as shown in Equation (1). Note that energy generation by power plant i in period k ($FS_{i,k}$) is constrained by its lower ($F_{i,LB}$) and upper bound of energy generation ($F_{i,UB}$), as demonstrated in Equation (2) and Equation (3), respectively. This section may be divided into subheadings. It should provide a concise and precise description of the experimental results, their interpretation, as well as the experimental conclusions that can be drawn.

$$\sum_i FS_{i,k} = D_k \qquad \forall k \tag{1}$$

$$FS_{i,k} \ \geq F_{i,LB} \times A_{i,k} \qquad \forall i \ \forall k \tag{2}$$

$$S_{i,k} \ \leq F_{i,UB} \times A_{i,k} \qquad \forall i \ \forall k \tag{3}$$

where $A_{i,k}$ is the binary variable for energy generation by power plant i in period k.

Next, the energy generation from power plant i in period k is subject to either its commissioning or decommissioning timeline, as demonstrated Equation (4). Energy generation from power plant i would only take place from the commissioning period (CM_i) onwards. Before the commissioning period, there should not be any energy generation from power plant i. By contrast, energy generation from power plant i would only take place until the period before the decommissioning period (DCM_i).

$$FS_{i,k} = \begin{cases} 0, & k < CM_i \\ 0, & k \geq DCM_i \end{cases} \qquad \forall i \ \forall k \tag{4}$$

Further, the energy generated from power plant i in period k should at least match its generation in the previous period, as shown in Equation (5). This constraint ensures a continuous operation of power plant i if it is selected for power generation. A temporary shutdown of power plant i would be impractical, thus resulting in a negative return on investment.

$$FS_{i,k+1} \ \geq FS_{i,k} \qquad \forall i \ ; \ k = 1, 2, \ldots, \ n-1 \tag{5}$$

CCS is one of the mitigation technologies that may be employed in power plant i for the satisfaction of the CO_2 emissions limits [36]. CDR via CCS decreases the CO_2 intensity of power plant i (CS_i). Therefore, the CO_2 intensity of power plant i with the deployment of CCS technology n in period k ($CR_{i,k,n}$) is calculated from Equation (6) [6]:

$$CR_{i,k,n} = \frac{CS_i \times (1 - RR_{k,n})}{1 - X_{k,n}} \qquad \forall i \ \forall k \ \forall n \tag{6}$$

where $RR_{k,n}$ and $X_{k,n}$ represent the removal ratio and parasitic power loss of CCS technology n in period k, respectively.

The deployment of CCS technology n is constrained by the upper bound of energy generation by power plant i, as shown in Equation (7). Further, the cumulative deployment of all CCS technologies should not exceed the energy generation by power plant i in period k, as demonstrated in Equation (8).

$$FR_{i,k,n} \ \leq F_{i,UB} \times B_{i,k,n} \qquad \forall i \ \forall k \ \forall n \tag{7}$$

$$\sum_n FR_{i,k,n} \leq FS_{i,k} \qquad \forall i \ \forall k \tag{8}$$

where $FR_{i,k,n}$ is the deployment of CCS technology n in power plant i in period k, and $B_{i,k,n}$ is the binary variable for the deployment of CCS technology n in power plant i in period k.

Like the energy generation from power plant i, the deployment of CCS technology n in power plant i in period k should at least match its deployment in the previous period, as shown in Equation (9). CCS technology is capital intensive. Therefore, it is not practical and is economically unviable for CCS technology n to be deployed in period k and not used in the subsequent period.

$$FR_{i,k+1,n} \ \geq FR_{i,k,n} \qquad \forall i \ \forall n \ ; \ k = 1, 2, \ldots, \ n-1 \tag{9}$$

CCS deployment incurs parasitic power loss of energy sources. Therefore, the net energy of power plant i after the deployment of CCS technology n in period k ($FNR_{i,k,n}$) is calculated from Equation (10):

$$FR_{i,k,n} \times (1 - X_{k,n}) = FNR_{i,k,n} \qquad \forall i \; \forall k \; \forall n \tag{10}$$

Aside from CCS, mitigation technologies that are available for power plant i in this work are alternative solid-based fuel s and alternative gas-based fuel g. Note that alternative solid and gas-based fuels may be used to replace fuels in power plant I, which are in solid and gas phases, respectively. The deployment of these alternative fuels in power plant i in period k should at least match their deployment in the previous period, as shown in Equations (11) and (12). The reasoning for this is the same as for CCS deployment.

$$FAS_{i,k+1,s} \; \geq FAS_{i,k,s} \qquad \forall i \; \forall s \; ; \; k = 1, 2, \ldots, \; n-1 \tag{11}$$

$$FAG_{i,k+1,g} \; \geq FAG_{i,k,g} \qquad \forall i \; \forall g \; ; \; k = 1, 2, \ldots, \; n-1 \tag{12}$$

where $FAS_{i,k,s}$ and $FAG_{i,k,g}$ are the deployment of alternative solid-based fuel s and gas-based fuel g in power plant i in period k, respectively.

Further, the deployment of alternative solid-based fuel s and gas-based fuel g in power plant i in period k is constrained by the upper bound of power generation by power plant i, as shown in Equations (13) and (14), respectively. The use of alternative fuels should never exceed the maximum power generation by power plant i, as these low-CO_2-intensity fuels are only purposed to replace the higher CO_2-intensity fuels that were originally deployed.

$$FAS_{i,k,s} \; \leq F_{i,UB} \times G_{i,k,s} \qquad \forall i \; \forall k \; \forall s \tag{13}$$

$$FAG_{i,k,g} \; \leq F_{i,UB} \times H_{i,k,g} \qquad \forall i \; \forall k \; \forall g \tag{14}$$

where $G_{i,k,s}$ and $H_{i,k,g}$ are the binary variables for the deployment of alternative solid-based fuel s and gas-based fuel g in power plant i in period k, respectively.

The cumulative deployment of all mitigation technologies available in this work should equate to the energy generated by power plant i in period k ($FS_{i,k}$), as demonstrated in Equation (15). The latter is initially determined from Equation (1).

$$FNS_{i,k} + \sum_{n} FR_{i,k,n} + \sum_{s} FAS_{i,k,s} + \sum_{g} FAG_{i,k,g} = FS_{i,k} \qquad \forall i \; \forall k \tag{15}$$

where $FNS_{i,k}$ is the net energy of power plant i without the deployment of mitigation technologies.

Other mitigation technologies that are available in this work are renewable energy source r, EP-NETs technology p and EC-NETs technology q. Note that these technologies are not plant-specific. Instead, the cumulative deployment of these mitigation technologies is determined for period k. The deployment of renewable energy source r ($FC_{k,r}$), EP-NETs technology p ($FEP_{k,p}$) and EC-NETs technology q ($FEC_{k,q}$) in period k are constrained by the availability of each technology, as demonstrated in Equation (16), Equation (17) and Equation (18), respectively:

$$FC_{k,r} \; \leq AC_{k,r} \times C_{k,r} \qquad \forall k \; \forall r \tag{16}$$

$$FEP_{k,p} \; \leq AEP_{k,p} \times D_{k,p} \qquad \forall k \; \forall p \tag{17}$$

$$FEC_{k,q} \; \leq AEC_{k,q} \times E_{k,q} \qquad \forall k \; \forall q \tag{18}$$

where $C_{k,r}$, $D_{k,p}$ and $E_{k,q}$ are the binary variables for the deployment of renewable energy source r, EP-NETs technology p and EC-NETs technology q in period k, respectively, and $AC_{k,r}$, $AEP_{k,p}$ and $AEC_{k,q}$ are the availabilities of renewable energy source r, EP-NETs technology p and EC-NETs technology q in period k, respectively.

Similar to the CCS and alternative fuels, the deployment of renewable energy source r, EP-NETs technology p and EC-NETs technology q in period k should at least match their deployment in the previous period, as demonstrated in Equation (19), Equation (20) and Equation (21), respectively. Should a plant be commissioned in period k, it is economically viable for its operation to be continuous in subsequent periods to ensure a positive return on investment.

$$FC_{k+1,r} \geq FC_{k,r} \qquad \forall r\ ;\ k = 1,2,\ldots,\ n-1 \tag{19}$$

$$FEP_{k+1,p} \geq FEP_{k,p} \qquad \forall p\ ;\ k = 1,2,\ldots,\ n-1 \tag{20}$$

$$FEQ_{k+1,q} \geq FEQ_{k,q} \qquad \forall q\ ;\ k = 1,2,\ldots,\ n-1 \tag{21}$$

The cumulative deployment of all mitigation technologies (CCS, alternative fuels, renewable energy sources and NETs) should satisfy the total demand of the energy system of period k; the latter includes the total power requirement (D_k) and that required by EC-NETs ($FEC_{k,q}$), as demonstrated in Equation (22):

$$\begin{aligned}\sum_i FNS_{i,k} + \sum_i\sum_n FNR_{i,k,n} + \sum_i\sum_s FAS_{i,k,s} + \sum_i\sum_g FAG_{i,k,g} \\ + \sum_r FC_{k,r} + \sum_p FEP_{k,p} = \sum_q FEC_{k,q} + D_k \qquad \forall k\end{aligned} \tag{22}$$

Following this, the total CO_2 load contribution from all power plants and mitigation technologies of energy planning period k (TE_k) is determined from Equation (23):

$$\begin{aligned}\sum_i FNS_{i,k}CS_i + \sum_i\sum_n FNR_{i,k,n}CR_{i,k,n} + \sum_i\sum_s FAS_{i,k,s}CIAS_{k,s} + \\ \sum_i\sum_g FAG_{i,k,g}CIAG_{k,g} + \sum_r FC_{k,r}CIC_{k,r} + \sum_p FEP_{k,p}CIEP_{k,p} \\ + \sum_q FEC_{k,q}\,CIEC_{k,q} = TE_k \quad \forall k\end{aligned} \tag{23}$$

where $CIAS_{k,s}$, $CIAG_{k,g}$, $CIC_{k,r}$, $CIEP_{k,p}$ and $CIEC_{k,q}$ represent the CO_2 intensities of alternative solid-based fuel s, alternative gas-based fuel g, renewable energy source r, EP-NETs technology p and EC-NETs technology q in period k, respectively.

Next, the total costs of power generation by power plant i in period k (CTF_k) are calculated from Equation (24). Whereas the first term of those equations represents the operating costs, the remaining two terms constitute the capital expenditure of the mitigation technologies. For capital expenditure, the second term relates to the fixed cost associated with the development of a new plant, e.g., land and machinery. Meanwhile, the third term is the fixed cost associated with the plant's capacity. A larger plant capacity would have a higher fixed cost, and vice versa.

$$FC_{k+1,r} \geq FC_{k,r} \qquad \forall r\ ;\ k = 1,2,\ldots,\ n-1 \tag{24}$$

where AFF is the annualized cost factor, and $OF_{i,k}$, $FC1_{i,k}$ and $FC2_{i,k}$ are the operational costs, fixed capital costs and capacity-dependent capital costs of power plant i in period k, respectively.

Following this, the total costs associated with the deployment of renewable energy source r (CTC_k), EP-NETs technology p ($CTEP_k$) and EC-NETs technology q ($CTEQ_k$) in period k are determined from Equation (25), Equation (26) and Equation (27), respectively:

$$\sum_r \begin{pmatrix} (FC_{k,r}\ OC_{k,r}) + (AFF.C_{k,r}\ CC1_{k,r}\ ) + \\ (AFF.FC_{k,r}CC2_{k,r}) \end{pmatrix} = CTC_k \quad \forall k \tag{25}$$

$$\sum_p \begin{pmatrix} \left(FEP_{k,p}\ OEP_{k,p}\right) + \left(AFF.D_{k,p}EPC1_{k,p}\right) + \\ \left(AFF.FEP_{k,p}EPC2_{k,p}\right) \end{pmatrix} = CTEP_k \quad \forall k \tag{26}$$

$$\sum_{q}\left(\begin{array}{c}\left(FEC_{k,q}\;OEC_{k,q}\right)+\left(AFF.E_{k,q}ECC1_{k,q}\right)+\\ \left(AFF\;.FEC_{k,q}ECC2_{k,q}\right)\end{array}\right)=CTEQ_{k}\quad\forall k \tag{27}$$

where $OC_{k,r}$, $OEP_{k,p}$ and $OEC_{k,q}$ are the operational costs of renewable energy source r, EP-NETs technology p and EC-NETs technology q in period k, respectively. Meanwhile, $CC1_{k,r}$, $EPC1_{k,p}$ and $ECC1_{k,q}$ are the fixed capital costs of renewable energy source r, EP-NETs technology p and EC-NETs technology q in period k, respectively. Further, $CC2_{k,r}$, $EPC2_{k,p}$ and $ECC2_{k,q}$ are the capacity-dependent capital costs of renewable energy source r, EP-NETs technology p and EC-NETs technology q in period k, respectively.

The total cost of the energy planning period k (TC_k) is calculated from Equation (28). Note that this calculation procedure considers all power plants and mitigation technologies, including those calculated from Equation (25), Equation (26) and Equation (27).

$$\begin{aligned}&CTF_{k}+\sum_{i}\sum_{n}(FNR_{i,k,n}\;CTR_{k,n}+AFF.CFR_{k,n}B_{i,k,n})\\&+\sum_{i}\sum_{s}(FAS_{i,k,s}\;CTAS_{k,s}+AFF.CFAS_{k,s}G_{i,k,s})\\&+\sum_{i}\sum_{g}\left(FAG_{i,k,g}\;CTAG_{k,g}+AFF.CFAG_{k,g}H_{i,k,g}\right)+\;CTC_{k}\\&+CTEP_{k}+CTEC_{k}=TC_{k}\quad\forall k\end{aligned} \tag{28}$$

where $CTR_{k,n}$ is the power generation cost with the deployment of CCS technology n in period k, and $CFR_{k,n}$, $CFAS_{k,s}$ and $CFAG_{k,g}$ are the fixed costs associated with the deployment of CCS technology n, alternative solid-based fuel s and gas-based fuels g in period k, respectively. Meanwhile, $CTAS_{k,s}$ and $CTAG_{k,g}$ are the costs of alternative solid-based fuel s and gas-based fuels g in period k, respectively.

Subsequently, Equations (29) and (30) present the constraints related to the total CO_2 emissions and total energy planning cost, respectively.

$$TE_{k}\;\leq L_{k}\qquad\forall k \tag{29}$$

$$TC_{k}\leq BD_{k}\quad\forall k \tag{30}$$

where BD_k is the budget allocation of energy planning period k.

The objective function of this work is set to minimise either the total energy planning cost (Equation (31)) or total CO_2 emissions (Equation (32)). If the former is selected as the objective function, the constraints from Equation (1) to Equation (29) ensure that the CO_2 emissions limit of a geographical region in period k is satisfied. Meanwhile, for the latter objective function, the constraints from Equation (1) to Equation (28) and Equation (30) limit the deployment of mitigation technologies subject to the budget availability of energy planning period k. Therefore, the CO_2 emissions limit may or may not be satisfied.

$$\min TC_{k} \tag{31}$$

$$\min TE_{k} \tag{32}$$

The presence of both continuous and integer variables results in the formulation being a MILP model. The mathematical formulation in this work is set up in Python, by using the open-source modelling language Pyomo [37]. The use of Pyomo allows users to freely use and modify the developed software. Additionally, this software may be utilised by all types of industries, as it is in a publicly available domain. Meanwhile, an easy-to-use input spreadsheet was developed in Microsoft Excel for the inclusion of the necessary energy planning data. The optimisation problem is solved to global optimality using the CPLEX solver from GAMS [38]; however, it can also be easily solved using open-source solvers such as CBC and Octeract [39]. In other words, one may not need access to GAMS for the use of the DECO2 software. Note that both CBC and Octeract are available in the public domain. The mathematical formulation of this work titled

'*Base_Model_Python.py*' is available on the *DECO2* GitHub page, which is accessible via https://github.com/mchlshort/DECO2 (accessed on 12 December 2022) or as a website hosted accessibly via www.deco2.nottingham.edu.my (hostname confirmed, website active on 1 March 2023). The next section presents the software infrastructure of the process integration-based software for optimal decarbonisation.

4. Software Infrastructure

The superstructural model formulation in this work is set up in Python, using the Pyomo algebraic modelling package, with an integrated user interface in Microsoft Excel, as demonstrated in Figure 2.

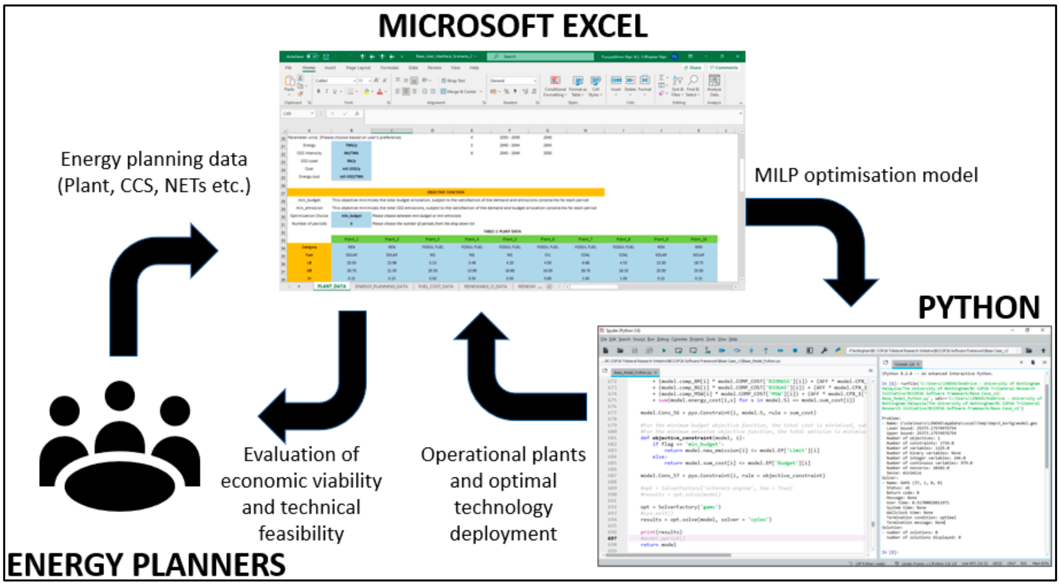

Figure 2. Software infrastructure.

The energy planning data that are required during optimisation are imported from the user interface file entitled '*Base_User_Interface.xlsx*', which was set up in Microsoft Excel. Besides creating a user-friendly tool, the inclusion of the energy planning data in a Microsoft Excel file allows energy planners without programming knowledge to utilise the software framework to carry out optimal decarbonisation. Note that fifteen sets of data must be included in the user interface file. Each tab in the user-interface file consists of data that must be included by energy planners before optimising the superstructural model in Python. Table 2 presents the energy planning information related to each tab in the user interface file.

As indicated in Table 2, the entries for all tabs (except '*TECH_IMPLEMENTATION_TIME*') in the user interface file consist of numerical values. However, the information in the '*TECH_IMPLEMENTATION_TIME*' tab is non-numerical. Instead, an energy planner needs to input the availabilities of the mitigation technologies in each period in terms of 'YES' (present) and 'NO' (absent). Upon inputting all energy planning data in the user interface file, an energy planner may choose the objective function from the '*PLANT_DATA*' tab, as shown in Figure 3.

Table 2. Energy planning information related to each tab in the user interface file.

Microsoft Excel Tab	Energy Planning Information
PLANT_DATA	Type of fuels, lower and upper bounds of power generation, CO_2 intensities, commissioning and decommissioning timeline of existing and upcoming power plants
ENERGY_PLANNING_DATA	Power demand, CO_2 emissions limit and budget availability in each energy planning period
FUEL_COST_DATA	Costs of fuels utilised in power plants in each energy planning period
RENEWABLE_CI_DATA	CO_2 intensities of available renewable energies in each energy planning period
RENEWABLE_COST_DATA	Costs of available renewable energies in each energy planning period
CAPEX_DATA_1	Fixed capital costs of mitigation technologies in each energy planning period
CAPEX_DATA_2	Capacity-dependent capital costs of mitigation technologies in each energy planning period
ALT_SOLID_CI	CO_2 intensities of alternative solid-based fuels in each energy planning period
ALT_SOLID_COST	Costs of alternative solid-based fuels in each energy planning period
ALT_GAS_CI	CO_2 intensities of alternative gas-based fuels in each energy planning period
ALT_GAS_COST	Costs of alternative gas-based fuels in each energy planning period
CCS_DATA	Removal ratios, parasitic power loss, power generation costs and fixed costs of CCS technologies in each energy planning period
NET_CI_DATA	CO_2 intensities of available NETs in each energy planning period
NET_COST_DATA	Costs of available NETs in each energy planning period
TECH_IMPLEMENTATION_TIME	The availabilities of mitigation technologies in each energy planning period

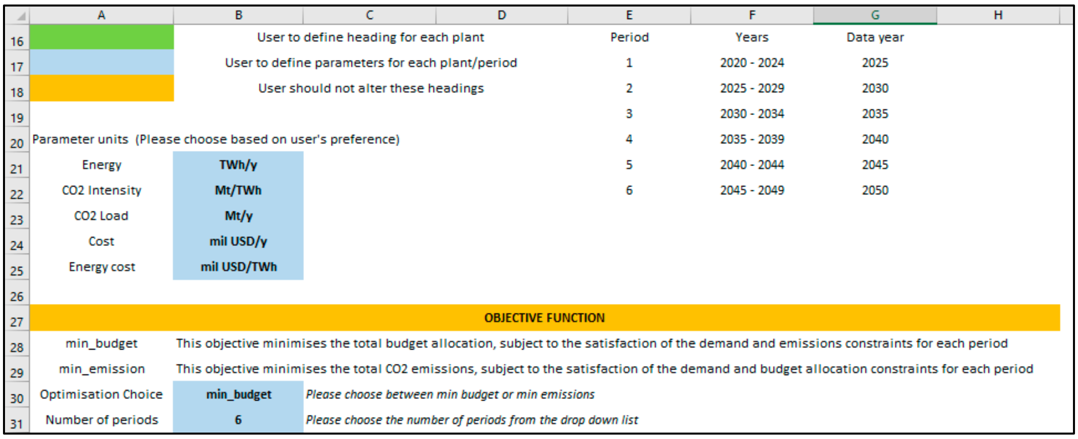

Figure 3. Snapshot of the 'PLANT_DATA' tab.

Based on Figure 3, cell 'B30′ presents the choices of objective functions available in this work. The available objective functions are *'min_budget'* (Equation (31)) and *'min_emission'* (Equation (32)). An energy planner may choose one of the objective functions depending on one's preference. Further, the energy planner may specify the number of energy planning periods based on the dropdown list in cell 'B31'. An energy planner may choose between 1 and 50 periods. Depending on the number of energy planning periods selected, an energy planner should input the energy planning data for the specified number of periods.

Next, an energy planner may optimise the superstructural model in the Python file entitled '*Base_Model_Python*'. Lines 692 and 694 of Figure 4 present the solver statement of the superstructural model, which makes use of the CPLEX solver from GAMS [38]. Note that a user may choose to alter the solver name on line 694 to any other suitable MILP solver if one does not have access to the CPLEX solver.

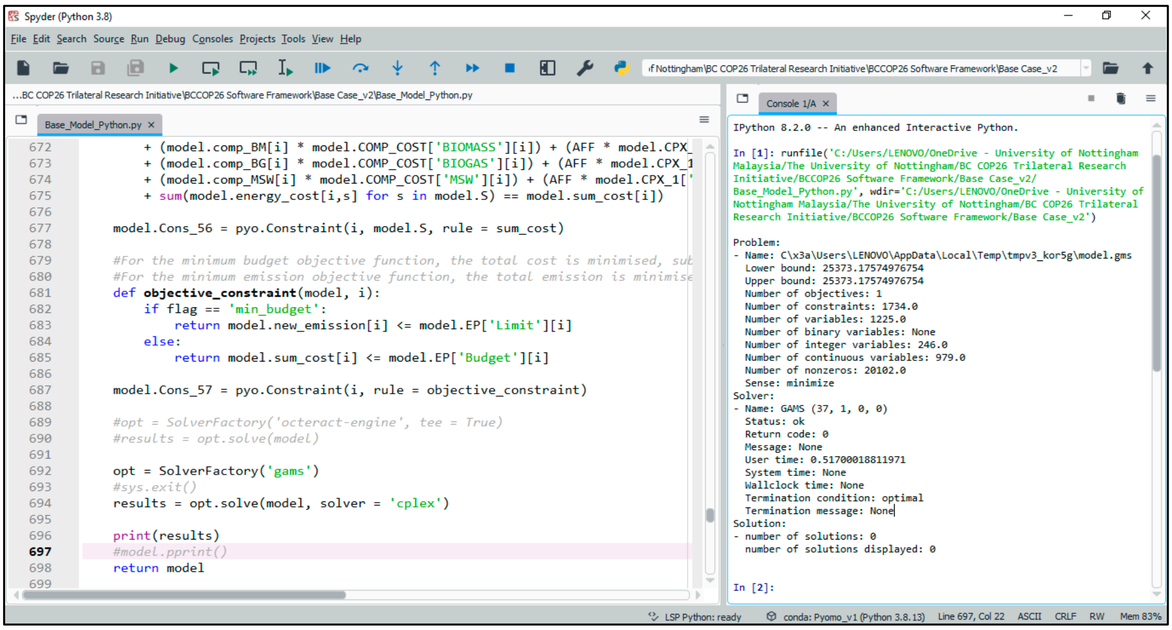

Figure 4. Optimising the superstructural model in Python.

Upon optimising the superstructural model, the console displays the solver status and parameters associated with an optimisation problem, e.g., the number of objectives, variables, user time, etc. If the termination condition is mentioned as 'optimal', it indicates that the superstructural model is solved to global optimality. An energy planner may now re-open the Microsoft Excel file to view results. Figure 5 presents the snapshot of the results in the user interface file.

	Fuel	Energy Generation	Energy	CI	CCS_1 CI	CCS_2 CI	CCS_1 Selection	CCS_2 Selection	CCS_1 Ret	CCS_2 Ret	Net Energy wo CCS	Net Energy w CCS_1
Plant_1	SOLAR	1	26.7	0.15	0.017	0.056	0	0	0	0	26.7	0
Plant_2	SOLAR	1	19.4	0.15	0.017	0.056	0	0	0	0	19.4	0
Plant_3	NG	1	20.5	0.5	0.056	0.188	0	0	0	0	0	0
Plant_4	NG	1	3.48	0.5	0.056	0.188	0	0	0	0	3.48	0
Plant_5	NG	1	8.08	0.5	0.056	0.188	0	0	0	0	8.08	0
Plant_6	OIL	0	0	0.8	0.089	0.3	0	0	0	0	0	0
Plant_7	COAL	0	0	1	0.111	0.375	0	0	0	0	0	0
Plant_8	COAL	1	18.1	1	0.111	0.375	0	0	0	0	0	0
Plant_9	SOLAR	1	20	0.15	0.017	0.056	0	0	0	0	20	0
Plant_10	SOLAR	1	18.75	0.15	0.017	0.056	0	0	0	0	18.75	0
EP_NET_1	EP_NET_1	1		-0.85								
EP_NET_2	EP_NET_2	0		-0.65								
EP_NET_3	EP_NET_3	0		-0.45								
EC_NET_1	EC_NET_1	1		-0.65								
EC_NET_2	EC_NET_2	0		-0.45								

ME1 ME2 ME3 ME4 ME5 ME6 MB1 MB2 MB3 MB4 MB5 MB6

Figure 5. Results snapshot of the optimised superstructural model.

Since six periods were chosen previously in Figure 3, an equivalent number of tabs were created in the user interface file, as shown in Figure 5. The results in Figure 5 consist of all power plants specified in the *'PLANT_DATA'* tab, as well as the available mitigation technologies. Table 3 describes the definition of the column heading in Figure 5.

Table 3. Energy planning information related to each tab in the user interface file.

Column Heading	Description
Fuel	Type of fuel used in the power plant
Gross Energy	Gross energy generated by each power plant
CCS_1 Ret	Energy from each power plant subjected to the deployment of CCS technology 1
CCS_2 Ret	Energy from each power plant subjected to the deployment of CCS technology 2
SOLID_1	Energy generation by alternative solid-based fuel type 1 in each power plant
SOLID_2	Energy generation by alternative solid-based fuel type 2 in each power plant
GAS_1	Energy generation by alternative gas-based fuel type 1 in each power plant
GAS_2	Energy generation by alternative gas-based fuel type 2 in each power plant
Net Energy	The net energy of each power plant and mitigation technology (NETs and renewable energy)
CO_2 *Load*	The total CO_2 load of each power plant and mitigation technology (NETs and renewable energy)
Cost	The total cost of the energy planning system

At this stage, an energy planner may analyse and evaluate the results to determine the practicality and ease of deployment of mitigation technologies. If any results are deemed unsuitable or overly optimistic, an energy planner may alter the energy planning data before re-running the optimisation software. Note that the energy planning may only need to alter the energy planning data, since all variables and constraints were specified in Python, with no inputs required from an energy planner.

The next section presents a case study that is used to demonstrate the optimal decarbonisation software framework.

5. Case Study

A hypothetical case study is used to demonstrate the application of the process integration-based software framework for optimal decarbonisation. The superstructural model in this work is demonstrated with six periods, each spanning a time interval of five years. Table 4 presents the energy planning data that are specified in the user interface file entitled *'Base_User_Interface.xlsx'*. Note that the data in Table 4 are assumed and do not represent any real-life scenario. These energy planning data, though not representative of an industrial scenario, would demonstrate the applicability of the software for optimal decarbonisation. The data in Table 4 are arranged in the order of the Microsoft Excel tabs mentioned in Table 2. Note that the data relevant to the *'TECH_IMPLEMENTATION_TIME'* tab are excluded for now.

Table 4. Energy planning information related to each tab in the user interface file.

Plant	Category	Fuel	Lower Bound (TWh y^{-1})	Upper Bound (TWh y^{-1})	CO_2 Intensity (Mt TWh^{-1})	CM_i	DCM_i
Plant 1	Renewable	Solar	20.03	26.70	0.15	1	7
Plant 2			15.98	21.30	0.15	1	7
Plant 3	Fossil Fuel	Natural Gas	5.13	20.50	0.50	1	7
Plant 4			3.48	13.90	0.50	1	7
Plant 5			4.20	16.80	0.50	1	7
Plant 6		Oil	4.00	16.00	0.80	1	3
Plant 7		Coal	6.68	26.70	1.00	1	5
Plant 8			4.53	18.10	1.00	1	7
Plant 9	Renewable	Solar	15.00	20.00	0.15	2	7
Plant 10			18.75	25.00	0.15	4	7

As shown in Table 4, there are 10 power plants available for power generation. Whereas the first eight plants are existing power plants (commissioned from Period 1 onwards), Plants 9 and 10 are upcoming power plants to be commissioned from Periods 2 and 4, respectively. In other words, Plants 9 and 10 would not be available for power generation before Periods 2 and 4, respectively. On the other hand, Plants 6 and 7, utilising oil and coal, respectively, would be decommissioned in Periods 3 and 5, respectively. Meanwhile, the lower bound of power generation by plants utilising renewable energy sources (Plants 1, 2, 9 and 10) is set to 75% of their upper bounds. In other words, the power generation from operational renewable-based power plants should at least be 75% of their maximum design capacity, since these plants cannot be ramped up easily to meet a sudden demand surge [40]. By contrast, power generation from plants utilising fossil-based sources may be ramped up quickly. Therefore, the lower bound for these plants (Plants 3 till 8) is set to 25% of their maximum generation capacity.

In Table 5, the energy planning is conducted based on incremental energy demand and stricter CO_2 emissions limits between successive periods. This scenario is often observed in developing countries with increasing populations, which leads to higher demand requirements. At the same time, lower CO_2 emissions limits are required for countries to meet their climate change targets. Note that the CO_2 emissions limit is observed to undergo a drastic decline at later periods. It is projected that the greater availability of mitigation technologies at later periods would make it relatively easier to drive CO_2 emissions reduction. Note that this work targets to achieve net-zero emissions by the final period, consistent with the pledges made at COP26 [35]. Further, economic growth contributes to a greater budget being available for energy planning across periods. Since the power plants in Table 4 make use of solar, natural gas, oil and coal, the associated fuel costs are presented in Table 6. As fossil-based sources are technologically matured, their costs are projected to remain stable for all periods [41,42]. By contrast, recent technological advancement has resulted in a significant decline in the cost of solar energy [43–45]. This information is captured in this work with the declining cost of solar energy in Table 6. Note that the cost decline in earlier periods is gradual, before increasing drastically towards later periods.

Table 5. Case study energy planning data: 'ENERGY_PLANNING_DATA'.

Energy Planning Parameters	1	2	3	4	5	6
Demand (TWh y^{-1})	60	75	90	105	120	135
CO_2 Emissions Limit (Mt)	20	18	15	11	6	0
Budget (mil USD y^{-1})	3000	3500	4000	4500	5000	5500

Table 6. Case study energy planning data: 'FUEL_COST_DATA'.

Fuel Cost (mil USD TWh^{-1})	1	2	3	4	5	6
Natural Gas	25					
Oil	49					
Coal	12					
Solar	40	35	25	13	8	3

Aside from the existing plants, this work also considers the potential deployment of renewable energies as separate plants for the mitigation of CO_2 emissions. The five renewable energies that are considered in this work are solar, hydropower, biomass, biogas and municipal solid waste (MSW). Each renewable energy differs in terms of CO_2 intensities (Table 7) and costs (Table 8). Like solar energy, the CO_2 intensities and costs of renewable energies are expected to decrease across periods [45,46]. In the final period, solar energy would be the cheapest [43,45] and has the lowest CO_2 intensity [19,47]. The superstructural model in this work would determine the optimal deployment of renewable energy sources (if necessary) to meet the demand and CO_2 emissions limits.

Table 7. Case study energy planning data: 'COMPENSATORY_CI_DATA'.

CO_2 Intensity of Renewable Energy (Mt TWh^{-1})	1	2	3	4	5	6
Solar	0.10	0.09	0.08	0.07	0.06	0.05
Hydropower	0.15	0.14	0.13	0.12	0.11	0.10
Biomass	0.30	0.28	0.26	0.24	0.22	0.20
Biogas	0.25	0.23	0.21	0.19	0.17	0.15
Municipal Solid Waste	0.30	0.29	0.28	0.27	0.26	0.25

Table 8. Case study energy planning data: 'COMPENSATORY_COST_DATA'.

Cost of Renewable Energy (mil USD TWh^{-1})	1	2	3	4	5	6
Solar	40	35	25	13	8	3
Hydropower	30	29	28	27	26	25
Biomass	20	18	16	14	12	10
Biogas	25	23	21	19	17	15
Municipal Solid Waste	20	19	18	17	16	15

Next, Tables 9 and 10 present the capital costs associated with all plants (fossil fuel, renewable and NETs). Note that this work assumes the capital expenditure for NETs plants to be higher than for fossil-based plants. Given that NETs are still in an early development phase with a lack of technological maturity, it is assumed that greater initial investment is required for NETs plants. However, the capital costs of all plants except fossil-based plants are expected to decrease across periods, with solar witnessing the largest decline. The capital costs for fossil-based plants are projected to remain constant, and their values are derived from the literature [41,42].

Table 9. Case study energy planning data: 'COMPENSATORY_CI_DATA'.

<table>
<tr><th>Fixed Capital Costs (mil USD TWh^{-1})</th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th><th>6</th></tr>
<tr><td>Natural Gas</td><td colspan="6" rowspan="3">400</td></tr>
<tr><td>Oil</td></tr>
<tr><td>Coal</td></tr>
<tr><td>Solar</td><td>400</td><td>350</td><td>300</td><td>250</td><td>200</td><td>150</td></tr>
<tr><td>Hydropower</td><td>400</td><td>380</td><td>360</td><td>340</td><td>320</td><td>300</td></tr>
<tr><td>Biogas</td><td rowspan="3">400</td><td rowspan="3">390</td><td rowspan="3">380</td><td rowspan="3">370</td><td rowspan="3">360</td><td rowspan="3">350</td></tr>
<tr><td>Biomass</td></tr>
<tr><td>Municipal Solid Waste</td></tr>
<tr><td>EP-NET 1</td><td rowspan="3">600</td><td rowspan="3">550</td><td rowspan="3">500</td><td rowspan="3">450</td><td rowspan="3">400</td><td rowspan="3">350</td></tr>
<tr><td>EP-NET 2</td></tr>
<tr><td>EP-NET 3</td></tr>
<tr><td>EC-NET 1</td><td rowspan="3">800</td><td rowspan="3">750</td><td rowspan="3">700</td><td rowspan="3">650</td><td rowspan="3">600</td><td rowspan="3">550</td></tr>
<tr><td>EC-NET 2</td></tr>
<tr><td>EC-NET 3</td></tr>
</table>

Table 10. Case study energy planning data: 'COMPENSATORY_CI_DATA'.

<table>
<tr><th>Fixed Capital Costs (mil USD TWh^{-1})</th><th>1</th><th>2</th><th>3</th><th>4</th><th>5</th><th>6</th></tr>
<tr><td>Natural Gas</td><td colspan="6" rowspan="3">100</td></tr>
<tr><td>Oil</td></tr>
<tr><td>Coal</td></tr>
<tr><td>Solar</td><td>100</td><td>85</td><td>70</td><td>55</td><td>40</td><td>25</td></tr>
<tr><td>Hydropower</td><td>100</td><td>90</td><td>80</td><td>70</td><td>60</td><td>50</td></tr>
<tr><td>Biogas</td><td rowspan="3">100</td><td rowspan="3">95</td><td rowspan="3">90</td><td rowspan="3">85</td><td rowspan="3">80</td><td rowspan="3">75</td></tr>
<tr><td>Biomass</td></tr>
<tr><td>Municipal Solid Waste</td></tr>
<tr><td>EP-NET 1</td><td rowspan="3">150</td><td rowspan="3">140</td><td rowspan="3">130</td><td rowspan="3">120</td><td rowspan="3">110</td><td rowspan="3">100</td></tr>
<tr><td>EP-NET 2</td></tr>
<tr><td>EP-NET 3</td></tr>
<tr><td>EC-NET 1</td><td rowspan="3">200</td><td rowspan="3">190</td><td rowspan="3">180</td><td rowspan="3">170</td><td rowspan="3">160</td><td rowspan="3">150</td></tr>
<tr><td>EC-NET 2</td></tr>
<tr><td>EC-NET 3</td></tr>
</table>

In this work, alternative solid (biomass) and gas-based fuels (biogas) are meant to replace coal and natural gas, respectively. For each fuel replacement, there are two types available for use. For example, the two choices of biomass could be an empty fruit bunch and a palm kernel shell [48]. Meanwhile, examples of biogas may be palm oil mill effluent [48] and animal manure [49]. In this work, it is assumed that the cheaper alternative fuel would have higher CO_2 intensity, and vice versa. The reasoning behind this assumption is that fuels with lower CO_2 intensity would often be subjected to processes with high operating costs. The CO_2 intensities and cost of the alternative fuels are presented in Tables 11–14. Once again, the improved energy efficiencies are projected to decrease the CO_2 intensities and costs of alternative fuels across periods.

Table 11. Case study energy planning data: 'ALT_SOLID_CI'.

CO_2 Intensity of Alternative Solid-Based Fuel (Mt TWh^{-1})	1	2	3	4	5	6
Technology 1	0.15	0.14	0.13	0.12	0.11	0.10
Technology 2	0.25	0.23	0.21	0.19	0.17	0.15

Table 12. Case study energy planning data: 'ALT_SOLID_COST'.

Cost of Alternative Solid-Based Fuel (Mt TWh^{-1})	1	2	3	4	5	6
Technology 1	20	19	18	17	16	15
Technology 2	15	14	13	12	11	10

Table 13. Case study energy planning data: 'ALT_GAS_COST'.

CO_2 Intensity of Alternative Gas-Based Fuel (Mt TWh^{-1})	1	2	3	4	5	6
Technology 1	0.15	0.14	0.13	0.12	0.11	0.10
Technology 2	0.25	0.23	0.21	0.19	0.17	0.15

Table 14. Case study energy planning data: 'ALT_GAS_CI'.

Cost of Alternative Gas-Based Fuel (Mt TWh^{-1})	1	2	3	4	5	6
Technology 1	35	34	33	32	31	30
Technology 2	30	29	28	27	26	25

Following this, the CCS data are presented in Table 15. Note that there are two CCS technologies available for deployment. Examples of CCS technologies are pre-combustion, post-combustion and oxyfuel capture [50]. In this work, these two CCS technologies may represent any of the available technologies. CCS technology 1 (e.g., pre-combustion capture) has a higher removal ratio and lower parasitic power loss in comparison to CCS technology 2 (e.g., post-combustion capture) [51,52]. Therefore, the latter has a lower cost in comparison to CCS technology 1. Due to the projected improvement in the technological maturity of CCS, the removal ratios of CCS systems are expected to increase. Meanwhile, the remaining CCS parameters (parasitic power loss and costs) are projected to decline across periods.

Finally, the CO_2 intensities and costs of NETs are presented in Tables 16 and 17, respectively. Note that both EP-NETs and EC-NETs are considered in this work, where each NET type is made up of three technologies. Some examples of EP-NETs are biochar and BECCS, whereas EC-NETs are made up of DAC and enhanced weathering. Note that NETs with the lowest CO_2 intensity (highest CDR capability) are the most expensive technology, and vice versa. Once again, like CCS technologies and renewable energy, all NETs are projected to mature across periods, resulting in declining CO_2 intensities and costs. The CO_2 intensities and costs of NETs are derived from the literature [53,54].

Table 15. Case study energy planning data: 'CCS_DATA'.

CCS Data	**1**	**2**	**3**	**4**	**5**	**6**
Removal ratio of CCS technology 1	0.85	0.86	0.87	0.88	0.89	0.90
Parasitic power loss of CCS technology 1	0.15	0.14	0.13	0.12	0.11	0.10
Power generation cost of CCS technology 1 (mil USD TWh^{-1})	34	33	32	31	30	29
Fixed cost of CCS technology 1 (mil USD TWh^{-1})	600	590	580	570	560	550
Removal ratio of CCS technology 1	0.65	0.66	0.67	0.68	0.69	0.70
Parasitic power loss of CCS technology 1	0.25	0.24	0.23	0.22	0.21	0.20
Power generation cost of CCS technology 2 (mil USD TWh^{-1})	29	28	27	26	25	24
Fixed cost of CCS technology 2 (mil USD TWh^{-1})	550	540	530	520	510	500

Table 16. Case study energy planning data: 'NET_CI_DATA'.

CO_2 Intensity of NETs (Mt TWh^{-1})	**1**	**2**	**3**	**4**	**5**	**6**
EP-NET 1	−0.80	−0.81	−0.82	−0.83	−0.84	−0.85
EP-NET 2	−0.60	−0.61	−0.62	−0.63	−0.64	−0.65
EP-NET 3	−0.40	−0.41	−0.42	−0.43	−0.44	−0.45
EC-NET 1	−0.60	−0.61	−0.62	−0.63	−0.64	−0.65
EC-NET 2	−0.40	−0.41	−0.42	−0.43	−0.44	−0.45
EC-NET 3	−0.20	−0.21	−0.22	−0.23	−0.24	−0.25

Table 17. Case study energy planning data: 'NET_CI_DATA'.

Cost of NETs (mil USD TWh^{-1})	**1**	**2**	**3**	**4**	**5**	**6**
EP-NET 1	43	41	39	37	35	33
EP-NET 2	40	38	36	34	32	30
EP-NET 3	37	35	33	31	29	27
EC-NET 1	49	47	45	43	41	39
EC-NET 2	37	35	33	31	29	27
EC-NET 3	24	22	20	18	16	14

Two scenarios are evaluated in this work using the hypothetical case study. The first scenario is considered the less ambitious approach toward mitigating CO_2 emissions. By contrast, the second scenario is more aggressive and ambitious in addressing climate change issues. The next section presents the details of Scenario 1.

5.1. Scenario 1

In Scenario 1, only certain mitigation technologies are available for CO_2 emissions mitigation, given as in Table 18.

Table 18. Availability of mitigation technologies in Scenario 1.

Technology Availability	1	2	3	4	5	6
Solar	✓	✓	✓	✓	✓	✓
Hydropower	✓	✓	✓	✓	✓	✓
Biomass	✓	✓	✓	✓	✓	✓
Biogas	✓	✓	✓	✓	✓	✓
MSW	✗	✗	✗	✓	✓	✓
Alternative solid-based fuel technology 1	✗	✗	✗	✗	✗	✗
Alternative solid-based fuel technology 2	✗	✗	✓	✓	✓	✓
Alternative gas-based fuel technology 1	✗	✗	✗	✗	✗	✗
Alternative gas-based fuel technology 2	✗	✗	✓	✓	✓	✓
CCS technology 1	✗	✗	✗	✗	✗	✗
CCS technology 2	✗	✗	✗	✓	✓	✓
EP-NET 1	✗	✗	✗	✗	✗	✗
EP-NET 2	✗	✗	✗	✗	✗	✗
EP-NET 3	✗	✗	✗	✗	✗	✗
EC-NET 1	✗	✗	✗	✗	✗	✗
EC-NET 2	✗	✗	✗	✗	✗	✗
EC-NET 3	✗	✗	✗	✗	✗	✗

Based on Table 18, all renewable energies (except MSW) are available for use in all energy planning periods. Note, however, that MSW is only available from Period 4. It is assumed that technology associated with MSW would take a longer time to mature [55]. In addition, one alternative solid- and gas-based fuel technology are unavailable in Scenario 1. These technologies are assumed to have lower CO_2 intensities (see Tables 11 and 13) and are far more mature as compared to their counterparts (technology 2). Therefore, only the less mature technologies of the alternative fuels are available for Scenario 1 and are only available from Period 3 onwards. The fuel substitution of coal and natural gas power plants would involve co-firing, thus requiring a retrofit to be carried out on both types of power plants. Retrofitting power plants is capital intensive and may not be available in earlier periods. A similar reasoning as to alternative fuels is applied for CCS. For the latter, only technology 2 is available from Period 4 onwards. Since CCS deployment is capital intensive, only one technology that has a lower removal ratio and higher parasitic power loss is available in Scenario 1. Finally, although NETs' deployment is crucial for CDR, its commercial deployment is not likely to be seen anytime soon [56]. Therefore, the deployment of NETs is absent in Scenario 1. The information in Table 5 is inputted in the *'TECH_IMPLEMENTATION_TIME'* tab in the user interface file entitled *'Base_User_Interface.xlsx'*.

5.1.1. Case 1

Once all energy planning information is included in the user interface file, optimisation is carried out using a superstructural model coded in the Python file entitled *'Base_Model_Python'*. The objective function of Case 1 is set to minimise the total CO_2 emissions (Equation (32)). In other words, the superstructural model is optimised subject to the budget availability in Table 5. Note that *'min_emission'* is selected in cell 'B30′ of the user interface file (see Figure 5). Figure 6 presents the results of Case 1. The detailed results of Case 1 in Scenario 1 are presented in Table S1 in the Supplementary Information.

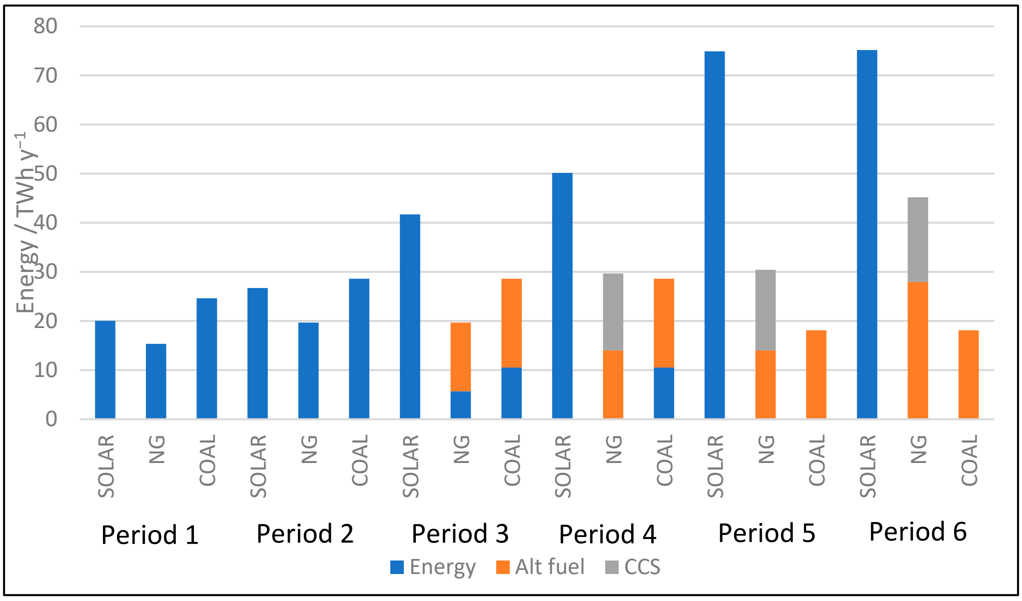

Figure 6. Power plants' configurations of Case 1 in Scenario 1.

Based on Figure 6, only power plants 1, 3, 7 and 8 were selected for power generation in Period 1. Among them, only one of them (power plant 1) is a solar plant (renewable energy). Although the power demand of 60 TWh y^{-1} was satisfied, the total CO_2 emissions were minimised at 35 Mt y^{-1}, thus violating the CO_2 emissions limit of 20 Mt y^{-1}. Moving on to Period 2, similar configurations as in Period 1 were observed, with additional power generation from the existing operational power plants. Once again, the power demand was satisfied, but the CO_2 emissions were violated by 24 Mt y^{-1} (= 42–18 Mt y^{-1}). The commissioning of solar-based power plant 9 in Period 2 meant that it is available for power generation in Period 3, and it was thus selected to satisfy the demand of 90 TWh y^{-1}. In addition to this, both biomass and biogas were deployed to replace the fuels in power plants 3 (natural gas) and 8 (coal), respectively. The alternative fuels have lower CO_2 intensities, thus contributing to lower cumulative CO_2 emissions of 29 Mt y^{-1}. Despite the higher costs of alternative fuels, their deployment is relatively cheaper than commissioning new power plants. Nevertheless, the CO_2 emissions limit was violated by 14 Mt y^{-1} (=29–15 Mt y^{-1}).

In Period 4, power plant 5, fueled by natural gas, was deployed to meet the incremental demand increase. However, its high CO_2 intensity increased the total CO_2 load, thus demanding additional mitigation measures. Therefore, both power plants 3 and 5 were retrofitted with CCS. The reduced power generation from those power plants is due to parasitic power losses during CCS deployment. Note that the CCS deployment in power plant 3 is in addition to its deployment of alternative gas-based fuel (biogas) technology 2. In other words, there were two mitigation technologies deployed for power plant 3. In addition to this, a new 3.45 TWh y^{-1} solar-based power plant that has a CO_2 intensity of 0.07 Mt TWh^{-1} was commissioned in Period 4. Note that the solar-based power plant 9 operated at its maximum capacity in Period 4. Despite additional mitigation measures and budget, the total CO_2 emissions in Period 4 were similar to Period 3. With the available budget, the total CO_2 could only be minimised to 29 Mt y^{-1}, thus violating the CO_2 emissions limit by 18 Mt y^{-1} (= 29–11 Mt y^{-1}).

Moving on to Period 5, power plant 7, which generated power from Period 1, was decommissioned (see Table 4). Therefore, solar-based power plant 10 was deployed to meet the incremental demand. Note that solar power plants 1, 9 and 10 were operating at their maximum capacity. The deployment of mitigation technologies (CCS and alternative fuels) in Period 5 was similar to those in Period 4. A similar situation was observed in the final period, except that natural gas-based power plant 4 was now deployed to satisfy the demand of 135 TWh y^{-1}. Note that CCS was deployed in power plant 4 for the mitigation of its emissions. Despite the deployment of several mitigation technologies, they were insufficient to satisfy the CO_2 emissions limits in all periods in Scenario 1. The results include fuel substitution to lower carbon alternatives, as well as the deployment of CCS. Without the deployment of NETs, the net-zero emissions target would not be achievable. However, this software fulfils the objective of deploying multiple mitigation technologies for achieving climate change targets.

5.1.2. Case 2

In Case 2, the total energy planning cost (Equation (31)) is minimised as the objective function. In other words, the CO_2 emissions limit for all periods must be satisfied. However, insufficient mitigation technologies (especially NETs) have resulted in an infeasible solution. In other words, CDR via NETs is necessary for the achievement of the net-zero target in the final energy planning period. Unless additional mitigation technologies are available, the CO_2 emissions limits in Scenario 1 would be constantly violated. Therefore, Scenario 2 is next investigated to identify the impact of additional mitigation technologies during energy planning.

5.2. Scenario 2

Scenario 2 is regarded to be more aggressive in comparison to Scenario 1, in which all mitigation technologies are now available for deployment (see Table 19). Unlike Scenario 1, some technologies are available at earlier periods due to an assumption of rapid technology maturity.

Table 19. Availability of mitigation technologies in Scenario 2.

Technology Availability	1	2	3	4	5	6
Solar	✓	✓	✓	✓	✓	✓
Hydropower	✓	✓	✓	✓	✓	✓
Biomass	✓	✓	✓	✓	✓	✓
Biogas	✓	✓	✓	✓	✓	✓
MSW	✗	✓	✓	✓	✓	✓
Alternative solid-based fuel technology 1	✗	✗	✓	✓	✓	✓
Alternative solid-based fuel technology 2	✗	✓	✓	✓	✓	✓
Alternative gas-based fuel technology 1	✗	✗	✓	✓	✓	✓
Alternative gas-based fuel technology 2	✗	✓	✓	✓	✓	✓
CCS technology 1	✗	✗	✗	✓	✓	✓
CCS technology 2	✗	✗	✓	✓	✓	✓
EP-NET 1	✗	✗	✗	✗	✓	✓
EP-NET 2	✗	✗	✗	✓	✓	✓
EP-NET 3	✗	✗	✓	✓	✓	✓
EC-NET 1	✗	✗	✗	✗	✓	✓
EC-NET 2	✗	✗	✗	✓	✓	✓
EC-NET 3	✗	✗	✓	✓	✓	✓

Based on Table 6, all renewable energies are available for deployment from Period 1 (except MSW, which is absent in Period 1). Both technologies of alternative solid- and gas-based fuels are available for deployment in Scenario 2, with their availability shown in Table 6. A similar situation also applied to both CCS technologies. Note that all NETs are now available for deployment, unlike in Scenario 1. Technology 3 of both NETs, having the highest CO_2 intensities versus technology 1 and 2, is available for deployment from Period 3 onwards. Meanwhile, technology 1 has the lowest CO_2 intensity (most effective for CDR) and is thus more mature compared to technology 2 and 3, but it is only available in the final two periods.

5.2.1. Case 1

The information in Table 6 is inputted in the *'TECH_IMPLEMENTATION_TIME'* tab in the Microsoft Excel-based user interface file entitled *'Base_User_Interface'*. Once again, the objective function of Case 1 is set to minimise the total CO_2 emissions (Equation (32)). Figure 7 presents the results of Case 1. The detailed results of Case 1 in Scenario 2 are presented in Table S2 in the Supplementary Information.

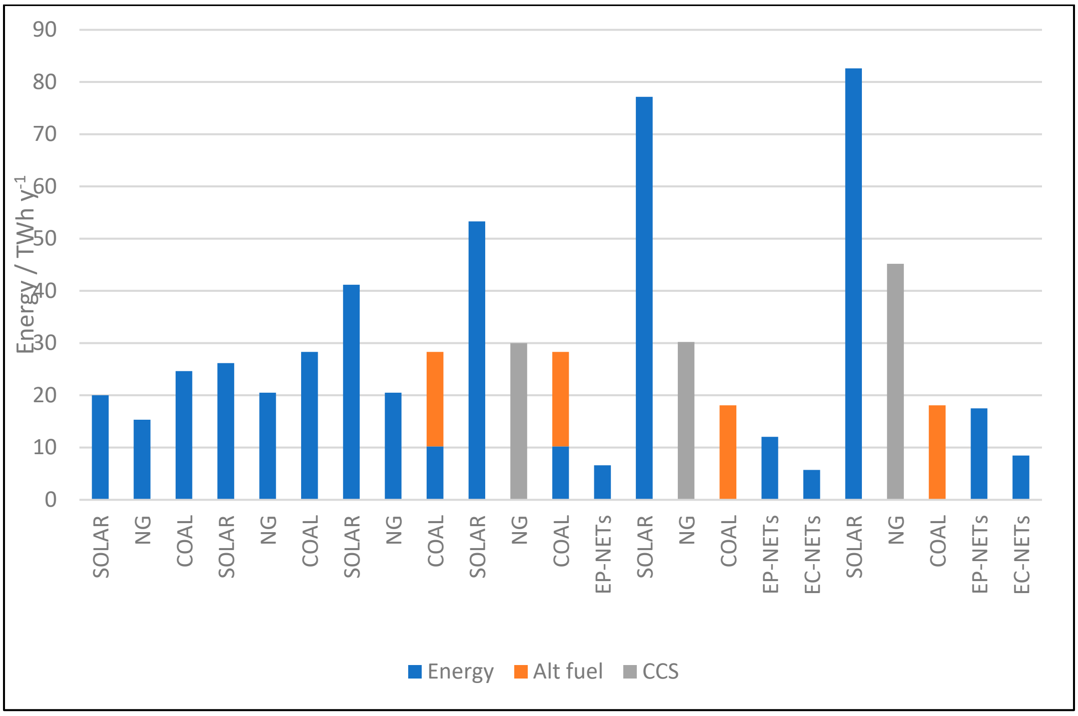

Figure 7. Power plants configurations of Case 1 in Scenario 2.

Based on Figure 7, the configurations of the power plants in Periods 1 and 2 were identical to those observed in Scenario 1. Therefore, the total CO_2 load in both Periods 1 and 2 was identical to Scenario 1, thus violating the CO_2 emissions limits. Moving on to Period 3, both technologies of alternative fuels and CCS technology 2 were available for deployment. Therefore, coal in power plant 8 was replaced with a lower-carbon alternative. In Scenario 1, the fuels in power plants 3 and 8 were both substituted with alternative fuel technology 2, which has higher CO_2 emissions but is cheaper. The use of the more expensive but cleaner alternative solid-based fuel technology 1 in power plant 8 meant there was an insufficient budget for fuel substitution to take place in power plant 3. Consequently, the CO_2 emission limit of 15 Mt y^{-1} in Period 3 was violated.

Period 4 saw the availability of all mitigation technologies, except for technology 1, concerning NETs. Like Scenario 1, CCS technology 2 was deployed for natural gas-based power plants 3 and 5. Additionally, 6.6 TWh y^{-1} of EP-NETs technology 2 was deployed to aid in CDR. Nevertheless, the total CO_2 load may only be minimised to 21 Mt y^{-1}, which is 10 Mt y^{-1} higher than the permissible limit. All mitigation technologies are available in the final two periods. The configurations of the power plants in Periods 5 and 6 were identical to those observed in Scenario 1. Aside from the deployment of CCS technology 2 and alternative solid-based fuel technology 1, EP-NETs technologies 1 and 2 and EC-NETs technology 1 were deployed. Technology 1 of both NETs was deployed due to their lower CO_2 intensities, thus contributing to a greater CDR. Note that the total CO_2 load in Period 5 was minimised at 5.9 Mt y^{-1}. This is the first period that saw the total CO_2 load below the CO_2 emissions limit of 6 Mt y^{-1}. Meanwhile, the net-zero emissions target was achieved in the final energy planning period. These results demonstrated that NETs' deployment is crucial to achieving relevant climate change targets. Additionally, these results also demonstrated the flexibility offered by the software in terms of making decisions between various technologies. Therefore, a user may input a practically unlimited number of technologies for making the business decision for driving decarbonisation initiatives. The ability of a user to customise the constraints and input parameters presents the key novelty of this work.

5.2.2. Case 2

Scenario 2 was repeated for Case 2 by minimising the total energy planning cost (Equation (31)) as the objective function. The presence of a greater pool of mitigation technologies made it possible to solve Case 2 to global optimality. Note that *'min_budget'* is selected in cell 'B30′ of the user interface file (see Figure 3). Figure 8 presents the results of Case 2. The detailed results of Case 2 in Scenario 2 are presented in Table S3 in the Supplementary Information.

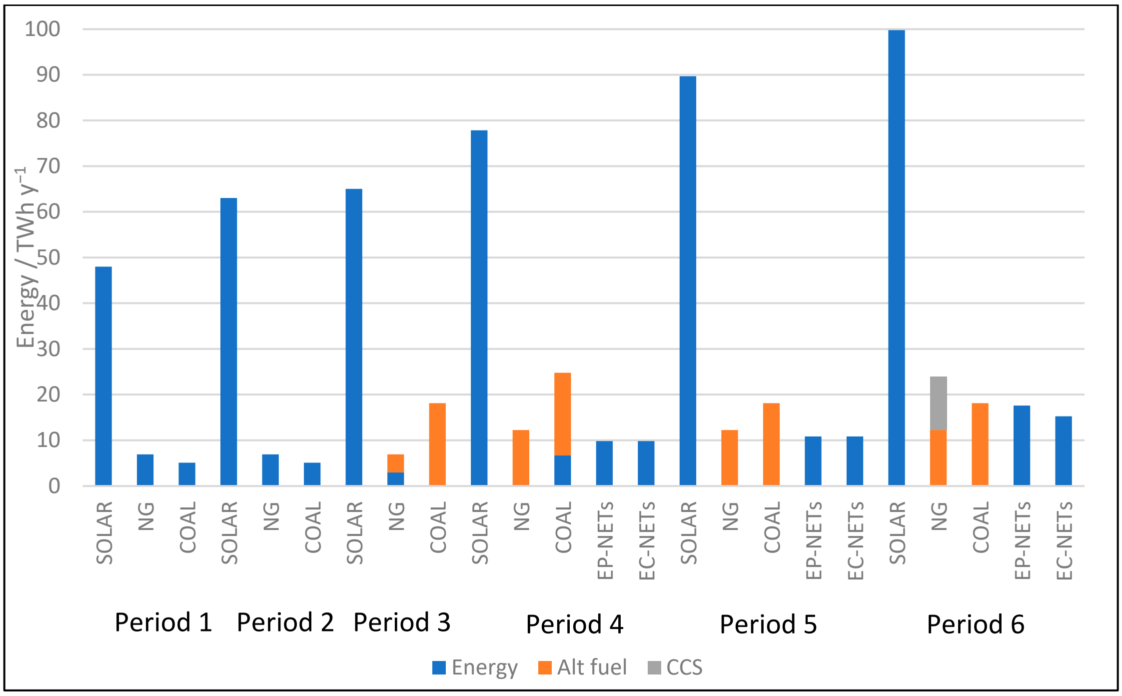

Figure 8. Power plants' configurations of Case 2 in Scenario 2.

Based on Figure 8, the CO_2 emissions limits for all periods were satisfied. In Period 1, solar-based power plants 1 and 2, natural gas-based plant 5 and coal-based plant 8 were operational. Unlike Case 1, the deployment of both renewable plants resulted in the total CO_2 load being slightly below the CO_2 emission limit, thus satisfying the constraint. Note, however, that the total cost amounted to USD 3673 mil y^{-1}, which is much higher than the allocated budget (USD 3000 mil y^{-1}). These results explain the violation of the CO_2 emissions limit in Period 1 of Case 1. A greater budget allocation is required to satisfy the emissions constraint in the latter case. Moving on to Period 2, solar-based power plant 9 was commissioned to meet the demand of 75 TWh y^{-1} and thus satisfy the CO_2 emissions limit of 18 Mt y^{-1}. Period 3 saw natural gas-based power plant 5 and coal-based plant 8 being substituted for a cleaner alternative. For both plants, technology 1 was deployed.

Note that co-firing of the alternative gas and natural gas-based fuels occurred in power plant 5.

Period 4 saw the deployment of NETs, combined with greater power generation from power plant 5. Instead of co-firing that occurred in Period 4, the natural gas-based plant 5 was completely substituted with alternative gas-based fuel technology 1. Note that technology 2 with lower CO_2 intensities was deployed for both types of NETs, despite being costlier. Since coal-based power plant 7 was decommissioned in Period 5, solar-fueled power plant 10 was deployed to meet the demand of 120 TWh y^{-1}. Period 6 saw the deployment of CCS technology 2 in power plant 4, fueled by natural gas as well as NETs technology 1. Once again, these results highlight the criticality of NETs' deployment in mitigating CO_2 emissions. These results demonstrate the novelty of this work, which takes into account both CCS and NETs and their importance in reducing GHG emissions. Over time, the software could be tailored to inputting novel technologies that would play a pivotal role in the power generation sector.

6. Discussion

The two scenarios have demonstrated the usefulness of the *DECO2* software in performing optimal decarbonisation for the power generation sector. The software can consider the various commissioning and decommissioning timelines among power plants. Additionally, the *DECO2* software can help drive and inform decarbonisation strategies that can consider fuel substitutions and the deployment of CCS as well as NETs. Although the problems demonstrated in this paper are small-scale problems only involving 10 power plants, the problem may very easily be scaled for optimal decarbonisation pathways to be conducted on a national scale. Both scenarios were solved to global optimality in negligible time, thus promoting the use of *DECO2* in the industry. Additionally, the *DECO2* software has highlighted the importance of CCS and NETs' deployment towards achieving the net-zero emissions targets and provides decisionmakers with a free-to-use, easily modifiable tool, as iterated by recent reports [4,57]. Additionally, the energy generation landscape would need to transition from fossil-based sources, i.e., coal, to alternative fuels, i.e., biomass. This would allow for existing energy infrastructure to be maintained while reducing GHG emissions. Most importantly, no single mitigation technology would be sufficient in achieving the relevant climate change targets, and hence, a portfolio optimisation approach is required. DECO2 provides a computing framework with which piecemeal data about individual component technologies can be integrated for effective decision support. However, the results obtained from this software are heavily dependent on input data and key parameters. This presents as one of the bottlenecks of the existing software framework. Therefore, data validation must be conducted to ensure that the obtained results would provide a significant meaning and direction in driving decarbonisation initiatives.

7. Conclusions

The *DECO2* optimal decarbonisation software framework was developed and introduced in this work to aid in carbon-constrained energy planning and the mitigation of CO_2 emissions. Consisting of a pool of available mitigation technologies such as alternative low-carbon fuels, renewable energies, CCS and NETs, the multiperiod energy planning model may be employed by policymakers and energy planners to determine the optimal deployment of each technology to meet the increasing power demand and stringent CO_2 emissions limits. The superstructural model in this work was developed in Python with an integrated user interface in Microsoft Excel. All energy planning data are inputted in the latter, as the former only serves as optimisation software, meaning that the model is simple to use. The open-source framework allows for the flexibility for advanced users to change the formulation and input their constraints. Two scenarios with different availabilities of mitigation technologies are investigated in this work to demonstrate the software's functionality. The first scenario, which is the least aggressive approach, is optimised based on the minimised emissions for each period. Note that none of the periods satisfied the CO_2

emissions limit due to an insufficient budget. Meanwhile, Scenario 2 is considered more aggressive due to the greater availability of mitigation technologies. For Case 1 in Scenario 2, the CO_2 emissions were violated in the earlier periods, before achieving the net-zero target in the final period. Meanwhile, the results of Case 2 in Scenario 2 demonstrated that early deployment of renewable energy is crucial to ensure that mitigations of CO_2 emissions at later periods can be performed with relative ease. Once NETs are available, their deployment is crucial to aid in CDR. Future work should focus on the demand variation on a small scale, i.e., daily, hourly, etc. The superstructural model developed in this work has the potential to deal with demand peaks within a small timeframe. Further, practical development in the associated mitigation technologies must be integrated into the existing model to build a realistic energy planning scenario. The software can also be improved to address the aforementioned data bottlenecks, which are inevitable when dealing with novel, unproven technologies.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/en16041708/s1, Table S1: Results for Case 1 in Scenario 1: (a) Period 1, (b) Period 2, (c) Period 3, (d) Period 4, (e) Period 5 and (f) Period 6; Table S2: Results for Case 1 in Scenario 2: (a) Period 1, (b) Period 2, (c) Period 3, (d) Period 4, (e) Period 5 and (f) Period 6; Table S3: Results for Case 2 in Scenario 2: (a) Period 1, (b) Period 2, (c) Period 3, (d) Period 4, (e) Period 5 and (f) Period 6.

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