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CHARACTERIZATION OF FUEL CELLS POWER DEMAND IN VEHICLES

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Abstract

The alternatives to internal combustion vehicles have arisen attention over the last years. Hydrogen, as an energy vector has multiple advantages, especially in heavy-duty vehicles. However, there is no simulator available to simulate the operation of fuel-cell (FC) vehicles. Thus, DLR-TT has devoted time to developing a phenomenological simulator for computing the power demand of a vehicle to accomplish a selected drive cycle and to calculate the FC unit power specifications.

The developed phenomenological model and simulator consider a hybrid FC / lithium-ion battery (LiB) power system, where the FC unit provides mostly steady state power, and the lithium-ion battery unit provides mostly dynamic power. Besides estimating the power demand, this model allows for the testing of different operating and design parameters concerning stability and power performance. The model was implemented in python in a well-structured manner to create in-house simulator.

In this thesis, the simulator was useful to run different drive cycles and find the most representatives for heavy-duty vehicles operating in Europe. Also, the properties of the vehicles, such as the powertrain efficiency, the aerodynamic characteristic, and the rotational inertia factor, were studied and it was possible to confirm that these are the parameters with the strongest effect on the power demand. The power split between FC and LiB units was also studied.

Another important point in this thesis was the evaluation of the power splitting strategy. The developed simulator was run to assess the optimum power contribution of the FC unit to the vehicle; the power was stepwise increased or decreased. It was concluded that for short cycles (ca. 1 h), there are advantages on having an increased capacity of the LiB unit.

Keywords: Hydrogen, fuel-cell, power demand, heavy-duty vehicles, lithium-ion battery

Resumo

As alternativas aos veículos de combustão têm vindo a ganhar importância ao longo dos últimos anos. Os veículos alimentados a hidrogénio apresentam múltiplas vantagens, especialmente na categoria dos veículos pesados. No entanto, ainda não se encontra disponível um simulador que permita simular a operação de carros a hidrogénio. Assim, a DLR-TT tem vindo a investir no desenvolvimento de um programa, que permita calcular a potência requerida, para que um veículo complete o ciclo de condução selecionado e estimar as especificações da célula de combustível.

O simulador considera que a célula de combustível opera juntamente com uma bateria, para garantir a produção da energia necessária, onde a célula de combustível é responsável pela produção de energia no estado estacionário e a bateria pela energia no estado dinâmico. Além de estimar a energia necessária, o simulador permite ainda testar diferentes parâmetros de operação e de projeto, de forma a avaliar a estabilidade e desempenho. Este modelo foi implementado em *Python* e estruturado de forma a ser utilizado na empresa.

Nesta tese, o simulador foi utilizado para simular diferentes ciclos de condução, no sentido de encontrar o mais característico da operação de veículos pesados na Europa. Além disso, foram testadas as propriedades do veículo, tais como a eficiência das transmissões, a velocidade aerodinâmica e o fator rotacional da inércia. Os resultados demonstraram que estes foram os quatro parâmetros com o efeito mais significativo na energia requerida. A estratégia de divisão da potência entre a FC e a bateria foi também estudada.

Outro ponto importante abordado nesta tese, foi a avaliação da estratégia de separação da energia. Recorreu-se ao simulador para encontrar a contribuição de potência ótima a realizar pela célula de combustível. Esta análise mostrou que, para curtas distâncias (aproximadamente 1 h), é vantajoso adotar baterias com maior capacidade e diminuir a potência produzida pela célula de combustível. Assim, quando a célula de combustível não gera uma corrente suficiente, a bateria pode ser trocada por outra com uma capacidade superior.

Palavras-chave:

Hidrogénio, célula de combustível, energia, veículos pesados, bateria

Declaration

I hereby declare, under the word of honour, that this work is original and that all non-original contributions are indicated, and due reference is given to the author and source.

Sign and date

Mara Filipa de Sousa Alves

Index

1	Introduction.....	1
1.1	Background and framing of the work	1
1.2	Presentation of the institution	2
1.3	Contributions of the author	2
1.4	Dissertation outline.....	2
2	Context and state of the art	3
2.1	Fuel cells (FC)	3
2.2	PEMFC	4
2.2.1	PEMFC components	4
2.2.2	PEMFC balance of plant (BoP).....	6
2.3	PEMFC thermodynamics and polarization curves	6
2.4	PEMFC applications	9
2.5	FC drive cycles	10
2.6	Computation of the power demand of the PEMFC.....	11
2.7	Existing simulators.....	13
2.8	PEMFC in hybrid systems	13
2.9	Hybrid system topology	14
3	Modelling and computer implementation	16
3.1	Simulator model structure	16
3.1.1	Mechanical simulation.....	16
3.1.2	Power splitting simulation	18
3.2	User interface	25
4	Results and discussion	26
4.1	Comparison of drive cycles and vehicles	26
4.2	A representative example.....	38
4.3	Hybrid strategy analysis	40
5	Conclusion.....	43

6	Assessment of the work done	44
6.1	Objectives achieved	44
6.2	Other work carried out	44
6.3	Final assessment	44
7	References	45
Appendix A -	Code example	50
Appendix B -	Default values for the vehicle's properties	52
Appendix C -	O ₂ and H ₂ moles stoichiometric	54
Appendix D -	Air compressor thermodynamics	56
Appendix E -	User interface	58
Appendix F -	Vehicle's properties effect	62
Appendix G -	Cycle's properties influence	80
Appendix H -	Example properties	84
Appendix I -	Current and potential evolution	86
Appendix J -	Operating conditions examples	88
Appendix K -	Battery capacity influence	92

List of Figures

Figure 2.1. Fuel unit cell representation and respective phenomena (extracted from [22]).	3
Figure 2.2. Single PEMFC structure (extracted from [22]).	4
Figure 2.3. MEA structure and schematic representation of gases, protons, and electrons transport in a PEMFC (extracted from [24]).	4
Figure 2.4. Representative example of a PEMFC BoP components: oxidant and fuel supply, and thermal and water management [29].	6
Figure 2.5. Graphical representation of the theoretical potential and real polarization curve of a PEMFC (adapted from [31]).	8
Figure 2.6. Representation of the forces that affect a vehicle moving to the right (adapted from [41]).	12
Figure 2.7. The basic structure of a PEMFC and battery hybrid system for vehicles application (adapted from [45]).	14
Figure 2.8. Fuel cell and battery hybrid system and current and potential distribution.	15
Figure 2.9. DC/DC converter device operation modes.	15
Figure 3.1. Representative scheme of the simulator logic structure: a) is the first stage - “mechanical simulation” and b) is the second stage - “power splitting simulation”.	16
Figure 3.2. W_{NET} , d and $W_{kinetic}$ evolution over time, and respective drive cycle.	17
Figure 3.3. Histogram with the drive cycle time fraction spent in each power range.	17
Figure 3.4. Power splitting approach used in the simulator to compute the $i_{Bat,HV}$, and $i_{FC,HV}$.	19
Figure 3.5. Polarization curves for a single FC and a FC stack.	20
Figure 3.6. Representation of the three possible changes in current demand: battery discharge (point 1), FC operates exclusively (points 2 and 3), and battery charges (point 4).	21
Figure 3.7. Fuel cell thermal management schematic representation.	24
Figure 4.1. Drive cycle representative of light-duty vehicles: speed (blue) and grade (yellow) evolution along time.	26
Figure 4.2. US drive cycles representative of heavy-duty vehicles: HHDDT, California, UDDS HD, and LHDC. Representation of speed (blue) and grade (yellow) evolution along time.	27
Figure 4.3. Power demand distinguished in power net and power kinetic recovery and respective evolution over time for the selected US drive cycles.	29
Figure 4.4. Histogram with the drive cycle time fraction spent in each power range for the four selected US cycles.	30

Figure 4.5. US drive cycles representative of heavy-duty vehicles: LH, urban, and RD. Representation of the speed (blue) and grade (yellow) evolution along time.	31
Figure 4.6. Representation of the power demand distinguished in power net and power kinetic recovery and respective evolution over time for the selected EU drive cycles.	33
Figure 4.7. Histogram with the drive cycle time fraction spent in each power range for the three selected EU cycles.	34
Figure 4.8. The NE and RE variation along each vehicle property variation aiming the analysis of the vehicle properties' effect on power demand considering the EU cycle (RD).	35
Figure 4.9. Graphical representation of the relation between the energy variation and the mass empty ($\Delta W_{\Delta \text{empty}}$) for different values of the cycle parameters: KPKE, $\tilde{a}$, v_{aero} , and k_i	36
Figure 4.10. Graphical representation of the relation between the energy variation and the vehicle frontal area ($\Delta W_{\Delta A_{\text{vehicle}}}$) for different values of the cycle parameters: KPKE, $\tilde{a}$, v_{aero} , and k_i	37
Figure 4.11. Power demand or produced and battery's SoC evolution over time for the HHDDT cycle, for an entire drive cycle and for a limited period.	38
Figure 4.12. Histogram with the drive cycle time fraction spent in each power range for the FC and battery.	39
Figure 4.13. Histogram with the drive cycle time fraction spent in each system efficiency range for the FC.	39
Figure 4.14. System efficiency and H_2 consumption contours assuming a battery capacity of 93 600 A s.	40
Figure 4.15. $T_{\min, \text{rated}}$ contours for different values of $\alpha +$ and $\alpha -$ assuming a battery capacity of 93 600 A s.	41
Figure 4.16. Energy demand from the FC and Battery for different values of $\alpha +$	41
Figure 4.17. Energy demand from the FC and Battery for different values of $\alpha -$	42
Figure 4.18. Time uncovered for different values of battery capacity, assuming constant $\alpha +$ and $\alpha -$ as 230 and 140 $A \cdot m^{-2} \cdot s^{-1}$, respectively.	42
Figure A.1. Example of the code developed in the project, responsible for the plot of the FC behaviour for different $\alpha +$ and $\alpha -$ values.	50
Figure A.2. Example of the code developed in the project, responsible for the plot of the FC behaviour for different $\alpha +$ and $\alpha -$ values.	51
Figure E.1. User interface regarding the mechanical simulation.	58
Figure E.2. User interface regarding the vehicle simulation.	59

Figure E.3. User interface regarding the power demand computation.	59
Figure E.4. User interface regarding the power splitting strategy.	60
Figure E.5. User interface regarding the power splitting strategy.	61
Figure F.1. Histogram with the drive cycle time spent in each power range for three different values of mass empty considering the US cycle (HHDDT).	62
Figure F.2. Histogram with the drive cycle time spent in each power range for three different values of mass load considering the US cycle (HHDDT).	63
Figure F.3. Histogram with the drive cycle time spent in each power range for three different values of rotational inertia factor considering the US cycle (HHDDT).	64
Figure F.4. Histogram with the drive cycle time spent in each power range for three different values of frontal area considering the US cycle (HHDDT).	65
Figure F.5. Histogram with the drive cycle time spent in each power range for three different values of drag coefficient considering the US cycle (HHDDT).	66
Figure F.6. Histogram with the drive cycle time spent in each power range for three different values of rolling coefficient considering the US cycle (HHDDT).	67
Figure F.7. Histogram with the drive cycle time spent in each power range for three different values of powertrain efficiency considering the US cycle (HHDDT).	68
Figure F.8. The NE and RE variation along each vehicle property variation aiming the analysis of the vehicle properties' effect on power demand considering the US cycle (HHDDT).	70
Figure F.9. Histogram with the drive cycle time spent in each power range for three different values of mass empty considering the EU cycle (RD).	71
Figure F.10. Histogram with the drive cycle time spent in each power range for three different values of mass load considering the EU cycle (RD).	72
Figure F.11. Histogram with the drive cycle time spent in each power range for three different values of inertial rotation factor considering the EU cycle (RD).	73
Figure F.12. Histogram with the drive cycle time spent in each power range for three different values of the frontal area considering the EU cycle (RD).	74
Figure F.13. Histogram with the drive cycle time spent in each power range for three different values of drag coefficient considering the EU cycle (RD).	75
Figure F.14. Histogram with the drive cycle time spent in each power range for three different values of rolling coefficient considering the EU cycle (RD).	76
Figure F.15. Histogram with the drive cycle time spent in each power range for three different values of powertrain efficiency considering the EU cycle (RD).	77

Figure G.1. Graphical representation of the relation between the energy variation and the mass empty ($\Delta W_{\Delta m_{empty}}$) for different values of the cycle parameters: PKE , $\tilde{a}$, $vaero$, and ki	80
Figure G.2. Graphical representation of the relation between the energy variation and the mass load ($\Delta W_{\Delta m_{payload}}$) for different values of the cycle parameters: $\tilde{a}$, PKE , $vaero$, and ki	80
Figure G.3. Graphical representation of the relation between the energy variation and the vehicle inertial rotation factor ($\Delta W_{\Delta e}$) for different values of the cycle parameters: PKE , $\tilde{a}$, $vaero$, and ki ...	81
Figure G.4. Graphical representation of the relation between the energy variation and the vehicle frontal area ($\Delta W_{\Delta A_{vehicle}}$) for different values of the cycle parameters: PKE , $\tilde{a}$, $vaero$, and ki	81
Figure G.5. Graphical representation of the relation between the energy variation and the vehicle rolling coefficient ($\Delta W_{\Delta CR}$) for different values of the cycle parameters: PKE , $\tilde{a}$, $vaero$, and ki	82
Figure G.6. Graphical representation of the relation between the energy variation and the vehicle drag coefficient ($\Delta W_{\Delta CD}$) for different values of the cycle parameters: PKE , $\tilde{a}$, $vaero$, and ki	82

Não foi encontrada nenhuma entrada do índice de ilustrações.

Figure I.1. Current density and cell potential evolution along time for the HHDDT cycle.	86
Figure I.2. W_{NET} , d and $W_{kinetic}$ evolution over time, and respective drive cycle.	86
Figure J.1. Power and SoC evolution along time for three examples with different values of $\alpha +$ and $\alpha -$: $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $120 \text{ A m}^{-2} \text{ s}^{-1}$ (a), $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $134 \text{ A m}^{-2} \text{ s}^{-1}$ (b), $220 \text{ A m}^{-2} \text{ s}^{-1}$ and $120 \text{ A m}^{-2} \text{ s}^{-1}$ (c).	88
Figure J.2. Histogram with the drive cycle time spent in each FC power range for three examples with different values of $\alpha +$ and $\alpha -$: $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $120 \text{ A m}^{-2} \text{ s}^{-1}$ (a), $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $134 \text{ A m}^{-2} \text{ s}^{-1}$ (b), $220 \text{ A m}^{-2} \text{ s}^{-1}$ and $120 \text{ A m}^{-2} \text{ s}^{-1}$ (c).	89
Figure J.3. Histogram with the drive cycle time spent in each battery power range for three examples with different values of $\alpha +$ and $\alpha -$: $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $120 \text{ A m}^{-2} \text{ s}^{-1}$ (a), $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $134 \text{ A m}^{-2} \text{ s}^{-1}$ (b), $220 \text{ A m}^{-2} \text{ s}^{-1}$ and $120 \text{ A m}^{-2} \text{ s}^{-1}$ (c).	90
Figure J.4. Histogram with the drive cycle time spent in each system efficiency range for three examples with different values of $\alpha +$ and $\alpha -$: $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $132 \text{ A m}^{-2} \text{ s}^{-1}$ (a), $250 \text{ A m}^{-2} \text{ s}^{-1}$ and $134 \text{ A m}^{-2} \text{ s}^{-1}$ (b), $220 \text{ A m}^{-2} \text{ s}^{-1}$ and $120 \text{ A m}^{-2} \text{ s}^{-1}$ (c).	90
Figure K.1. System efficiency, and H_2 consumption for different values of battery capacity assuming constant $\alpha +$ and $\alpha -$ as 230 and $140 \text{ A m}^{-2} \text{ s}^{-1}$, respectively.	92

Figure K.2. $T_{min, rated}$ for different values of battery capacity, assuming constant $\alpha +$ and $\alpha -$ as 230 and $140 \text{ A m}^{-2} \text{ s}^{-1}$, respectively. 92

List of Tables

<i>Table 3.1. Battery input parameters and respective default values.....</i>	<i>18</i>
<i>Table 3.2. Hybrid system strategy input parameters and respective default values.....</i>	<i>19</i>
<i>Table 4.1. Kinetic parameters computed by the simulator for the US selected cycles: HHDDT, California, UDDS HD, and LHDC.....</i>	<i>28</i>
<i>Table 4.2. Average net power demand and recoverable power produced for each selected US cycle.</i>	<i>30</i>
<i>Table 4.3. Kinetic parameters computed by the simulator for the EU selected cycles: LH, urban, and RD.</i>	<i>32</i>
<i>Table 4.4. Average net power demand (NP) and recoverable power produced (RP) for each selected EU cycle.</i>	<i>33</i>
 <i>Table B.1. Default values and respective references for vehicle properties.</i>	 <i>52</i>
 <i>Table F.1. Values of NE and RE for different values of vehicle mass empty considering the US cycle (HHDDT).</i>	 <i>62</i>
<i>Table F.2. Values of NE and RE for different values of vehicle mass load considering the US cycle (HHDDT).</i>	<i>63</i>
<i>Table F.3. Values of NE and RE for different values of vehicle inertial rotation factor considering the US cycle (HHDDT).</i>	<i>64</i>
<i>Table F.4. Values of NE and RE for different values of vehicle frontal area considering the US cycle (HHDDT).</i>	<i>65</i>
<i>Table F.5. Values of NE and RE for different values of vehicle drag coefficient considering the US cycle (HHDDT).</i>	<i>66</i>
<i>Table F.6. Values of NE and RE for different values of vehicle rolling coefficient considering the US cycle (HHDDT).</i>	<i>67</i>
<i>Table F.7. Values of NE and RE for different values of vehicle powertrain efficiency considering the US cycle (HHDDT).</i>	<i>68</i>
<i>Table F.8. Values of NE and RE for different values of vehicle converter efficiency considering the US cycle (HHDDT).</i>	<i>69</i>
<i>Table F.9. Values of NE and RE for different values of vehicle mass empty considering the EU cycle (RD).</i>	<i>71</i>
<i>Table F.10. Values of NE and RE for different values of vehicle mass load considering the EU cycle (RD).</i>	<i>72</i>

<i>Table F.11. Values of NE and RE for different values of vehicle inertial rotation factor considering the EU cycle (RD).</i>	73
<i>Table F.12. Values of NE and RE for different values of vehicle frontal area considering the EU cycle (RD).</i>	74
<i>Table F.13. Values of NE and RE for different values of vehicle drag coefficient considering the EU cycle (RD).</i>	75
<i>Table F.14. Values of NE and RE for different values of vehicle rolling coefficient considering the EU cycle (RD).</i>	76
<i>Table F.15. Values of NE and RE for different values of vehicle powertrain efficiency considering the EU cycle (RD).</i>	77
<i>Table F.16. Values of NE and RE for different values of vehicle converter efficiency considering the EU cycle (RD).</i>	78
 <i>Table H.1. FC and battery properties defined for the representative example simulation.</i>	 84
 <i>Table J.1. Operating conditions for three different examples.</i>	 88
<i>Table J.2. $T_{min, rated}$ and H_2 consumption for three examples with different values of $\alpha +$ and $\alpha -$: a - (250 and 132) $A\ m^{-2}\ s^{-1}$, b - (250 and 160) $A\ m^{-2}\ s^{-1}$, c - (220 and 120) $A\ m^{-2}\ s^{-1}$.</i>	91

Notation and Glossary

A	Area	m^2
a	Acceleration	m s^{-2}
$\tilde{a}$	Characteristic acceleration	m s^{-2}
C	Capacity	A s
C_D	Drag resistance coefficient	
C_p	Specific heat capacity	$\text{J K}^{-1} \text{kg}^{-1}$
C_R	Rolling resistance coefficient	
D	Distance	m
d	Parameters variation	%
e	Rotational inertia factor	
F	Faraday's constant	$96\,485 \text{ C mol}^{-1}$
G	Gibbs free energy	J
g	Gravitational constant	m s^{-2}
h	Enthalpy	J
i	Current	A
J	Current density	A m^{-2}
ki	Kinetic intensity	s^{-1}
l	Height	m
M	Mass molar	kg s^{-1}
m	Mass	kg
$\dot{m}$	Mass consumption rate	kg s^{-1}
n	Number of moles	mol
$\dot{n}$	Molar consumption rate	mol s^{-1}
N_C	Number of fuel cells	
N_E	Net energy	kW h
N_P	Net power	kW
P	Pressure	Pa
K_{PKE}	Positive kinetic energy	m s^{-2}
p	Partial pressure	
Q	Moving charge	C
$\dot{Q}$	Heat	W
$\dot{Q}_{QDT}$	Heat rejection capacity	W K^{-1}
R	Resistivity per surface area	Ωm^2
r	Resistance	Ω
R_E	Recoverable energy	kW h
R_P	Recoverable power	kW
S	Entropy	J K^{-1}
S_{SoC}	Battery's state of charge	
T	Temperature	K
t	Time	s
U	Potential	V
V	Volume	m^3
v	Speed	m s^{-1}
W	Energy	J
$\dot{W}$	Power	W

Greek Letter's

α	Current variation per time unit	$\text{A cm}^{-2} \text{s}^{-1}$
β	Charge transfer coefficient	
ε	Efficiency	
θ	Pitch angle of the hillside	
η	Isentropic efficiency	

μ	Potential losses	
ρ	Density	kg m^{-3}
$\mathcal{R}$	Gas constant	$8.314 \text{ J mol}^{-1} \text{ K}^{-1}$
χ	Molar fraction	
γ	Heat capacity ratio	

Indexes

$^{\circ}$	Standard state reversible conditions
o	FC's i and U values of the polarization curve's reference point
$+$	Current increasing per time unit
$-$	Current decreasing per time unit
act	Activation overpotential
aero	Aerodynamic speed
air	Air's density and specific heat capacity
air,cathode	Air's mass consumption rate in the cathode
Bat	Battery's C and r or LV side battery's W , $\dot{W}$, i and U demand
Bat,n	Previous battery's potential demand
Bat,HV	Battery's current and potential demand in the HV side
cathode	Cathode's in flow and compressor's out flow P and Cathode's γ
char,max	Maximum battery's current absorbed during a certain period
climb	Gravitational resistance power
coolant	Coolant's mass consumption rate and C_p
comp	Air compressor's isentropic efficiency
computed	Radiator's QDT computed
conc	Concentration losses
cycle	Cycle's distance
DC/DC	DC/DC converter's efficiency
dis,max	Maximum battery's current release during a certain period
drag	Drag resistance power
E	Exchange current density
e^{-}	e^{-} moles transferred
elec	Electrical work
empty	Truck empty mass
ext	Environment's T
FC	FC's R , A , i and U demand in the LV side, heat loss, and ε
FC,n	Previous FC's current demand in the LV side
FC, BoP	FC's current produced for the BoP
FC, Bruto	FC's bruto current produced
FC, comp	FC's current and power produced to the air compressor
FC,H ₂	H ₂ moles consumption in a single FC
FC,HV	FC's current and potential demand in the HV side
FC,HV,max	Maximum FC current demand increase in the HV side
FC,HV,min	Maximum FC current demand decrease in the HV side
FC,max	Maximum FC current demand increase in the LV side
FC,min	Maximum FC current demand decrease in the LV side
FC,NET	FC's net current produced
FC,O ₂	O ₂ moles consumption in a single FC
H ₂	H ₂ moles consumption in a FC stack and H ₂ partial pressure
H ₂ , anode	H ₂ n in the FC stack's anode
H ₂ , st	H ₂ stiochiometric feed flow rate
H ₂ O	H ₂ O partial pressure
HV	Current or potential in the DC/DC converter's high potential side
In,coolant	Coolant in flow's temperature
in,comp	Air compressor in flow's pressure and temperature
inertia	Rotational inertia resistance power

kinetic	Recoverable mechanical energy and power
kpi	Radiator's <i>QDT</i> defined by the user
L	Limit current density
LV	Current or potential in the DC/DC converter's low potential side
max	Battery's maximum SoC and radiator's T variation
mech	Total mechanical power
min	Battery's minimum state of charge
min,rated	Minimum FC's operating T
n	Previous battery's SoC
n+1	New battery's SoC
NET	Net mechanical power and energy demand
NET, d	Real net mechanical power and energy demand
O ₂	O ₂ moles consumption in a FC stack and O ₂ partial pressure
O ₂ , air	O ₂ 's mole fraction in the air
O ₂ , cathode	O ₂ $\dot{n}$ in the FC stack's cathode, and O ₂ 's mass molar
ohmic	Ohmic losses and resistance
out, air	Gas out flow's temperature
out,coolant	Coolant out flow's temperature
out,comp	Air compressor out flow's pressure and temperature
out,H ₂	H ₂ out flow's temperature
out,radiator	Radiator out flow's temperature
PT	Powertrain efficiency
payload	Truck payload mass
rated	Ideal FC's operating T
rol	Rolling resistance power
system	System efficiency
stack	Coolant's T variation
teo	Theoretical FC's potential
vehicle	Vehicle's cross-sectional area

List of Acronyms

AFC	Alkaline fuel cell
BoP	Balance of plant
CL	Catalyst layer
FC	Fuel cell
FCV	Fuel cell vehicles
GDL	Gas diffusion layer
GHG	Greenhouse gases
HDV	Heavy-duty vehicles
HHDDT	California Air Resources Board Heavy Heavy-Duty Diesel Truck
HV	High- potential converter's side
icct	International Council on Clean Transportation
LDV	Light-duty vehicles
LH	VECTO Long Haul cycle
LHDC	Long Haul Drive Cycle
LiB	Lithium-ion battery
LV	Low- potential converter's side
MCFC	Molten carbonate fuel cell
MEA	Membrane electrode assembly
PAFC	Phosphoric acid fuel cell
PEMFC	Proton exchange electrolyte membrane fuel cell
PTFE	Polytetrafluoroethylene
RD	VECTO Regional Delivery cycle
SoC	State of charge
SOFC	Solid oxide fuel cell

UDDS HD Urban Dynamometer Driving Schedule for Heavy-Duty Vehicles

1 Introduction

1.1 Background and framing of the work

One of the critical topics under investigation today is climate change. Consequently, environmental issues have gained increasing attention and prominence [1-5]. In fact, fossil fuels remain the most relevant contributor to world energy demand, representing around 81 % of the world's annual energy production in 2019, which results in intense CO₂ emissions [6].

In Europe, 25 % of greenhouse gas (GHG) emissions result from the transport sector. For that reason, the European Union has agreed to define targets to lower GHG emissions in the transport sector by at least 60 % below the 1990 levels by 2050 [7].

Light-duty vehicles represent over 62 % of the transport's CO₂ emissions in Europe [5, 8]. Thus, as an efficacious attempt to thwart this increment in GHG emissions, multiple car brands have found several solutions, such as hybrid electric vehicles, electric vehicles, and fuel cell vehicles (FCV). However, electric vehicles have shown better outcomes since the hybrid ones release still some pollutants into the air and the FCVs exhibit high costs and low durability [9].

Even though the light-duty vehicles represent the predominant part of the emissions, the heavy-duty vehicles also represent a significant part. In 2015, heavy-duty vehicles were responsible for over 25 % of the transport's CO₂ emissions [10]. Thus, the attention devoted to this category has arisen. In this vehicle sector, the battery used in electric vehicles seems to not be an effective alternative to fossil fuels due to its low energy density and long charging times [11].

On the other hand, the FCV has proven to bring a powerful environmental benefit, particularly when hydrogen is generated employing renewable energy sources [10]. Additionally, the FCVs are characterized by their low operating temperatures, high energy-conversion efficiency, short start-up times, quiet operation, low emission, compactness and fast load response [11-14].

Still, extreme power demand variations lead to fuel cell (FC) degradation. Thus, an FC-battery system can be advantageous [10]. It provides the hybrid system with a fast answer to load variations, higher power production values, and reduced hydrogen consumption [11].

Currently, commercial simulators, such as FASTSim and VECTO, has already been developed to analyse vehicles' power demands, fuel consumption, and CO₂ emissions based on the target speed evolution along time (drive-cycles). However, neither of them is adapted to European hybrid Battery-FC vehicles. The first one is tailored for different US electric and hybrid vehicles' driving analyses, while the second was developed by the European Commission to evaluate the heavy-duty vehicles' CO₂ emissions [15-17].

Therefore, one goal of this thesis was to actively contribute for the development of a new simulator to study and evaluate the hybrid-vehicles power splitting strategy in Europe.

In this regard, the second goal of this thesis was to use the model implemented to evaluate how the properties of the FC and battery can be adjusted to result in the optimization of the hybrid vehicles. Thus, several simulations were ran using the simulator developed.

1.2 Presentation of the institution

The work discussed on this thesis was carried out at the German Aerospace Center (DLR) in the Institute of Engineering Thermodynamics (DLR-TT) in Stuttgart. This research centre focuses on diverse sectors such as aviation, space travel, energy, traffic, security, and digitalization [18, 19]. One of DLR's points of attention is hydrogen as one energy source. Thus, multiple research projects are being carried out to study the FCs implementation in cars, aircraft, ships, and buses [18,19].

1.3 Contributions of the author

The work presented in this thesis was conducted focusing on the development of a simulator to characterize the power demand in FC-battery hybrid vehicles for further development of stressor tests. It was done at DLR, where some previous work had already been done.

A significant part of the core structure of the simulator had been written by Dr Juan Monreal Sanchez. My contribution included the development of around 15 % of the total code (3500 lines), the review of the entire code, and the development of a user-friendly interface.

On top of that, I did an intense evaluation of the existing drive cycles and added a model to the simulator to include the VECTO cycles. The vehicle's properties were also analysed by me, as well as the FC efficiencies and hybrid strategy.

1.4 Dissertation outline

This dissertation was organized into six conventional chapters. The introduction frames the thesis' context and purpose. This first chapter is followed by the context and state of the art, where the actual knowledge about fuel cell technology is discussed.

After that, the developed simulator is explained in the computer application's chapter. The results attained with the simulator are evaluated in the subsequent chapter - Results and Discussion.

Lastly, the thesis finishes with the conclusions and the assessment of the work chapters. At this final chapter, a detailed global review of the project can be found.

2 Context and state of the art

2.1 Fuel cells (FC)

FCs are widely known as electrochemical energy converters. They are responsible for the chemical energy's direct transformation into electric energy. The chemical energy outcomes from redox reactions between the fuel and the oxidizing agent [20].

An FC structure assembles an electrolyte layer in the middle of an anode and a cathode, as shown in Figure 2.1 [21, 22].

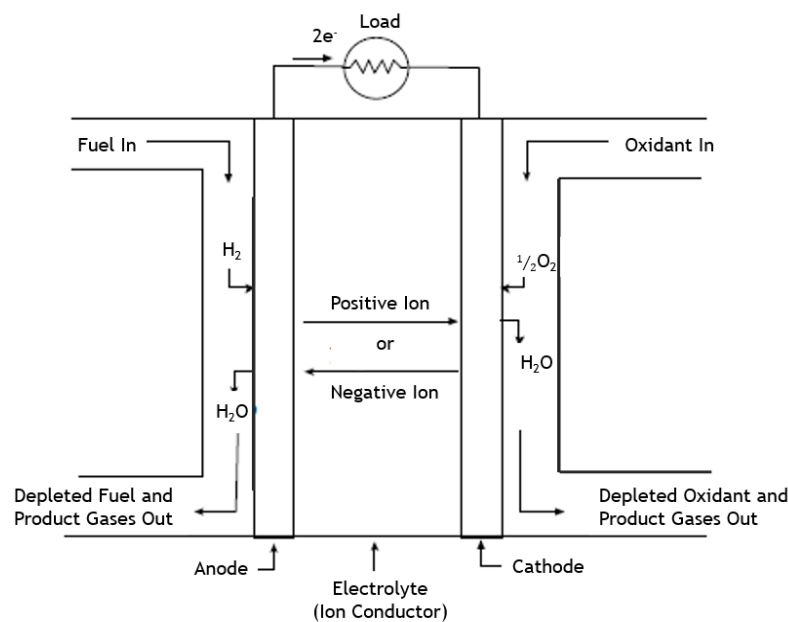


Figure 2.1. Fuel unit cell representation and respective phenomena (extracted from [22]).

Continuously, a fuel stream is fed to the anode, and an oxidant stream is fed to the cathode. In this unit cell, the redox reaction takes place at the electrode, producing an electric current through the external circuit. Besides electricity, water and heat are also produced [21].

FCs are often categorized based on the type of electrolyte used in the cells. There are five main types: the proton exchange electrolyte membrane fuel cell (PEMFC), the alkaline fuel cell (AFC), the phosphoric acid fuel cell (PAFC), the molten carbonate fuel cell (MCFC), and the solid oxide fuel cell (SOFC) [23].

The operating temperature is a determinant factor in the FC system. At low operating temperatures, the anode catalyst is strongly poisoned by CO [21]. Thus, choosing the fuel type according to the operating temperature is crucial. AFC, PEMFC and PAFC are considered low-temperature FCs, while high-temperature ones comprise SOFC and MCFC [23].

2.2 PEMFC

The PEMFCs are characterized by their proton exchange membrane. This type of FC produces electricity from the chemical reaction between hydrogen (H_2) and oxygen (O_2) (Equation (2.1)). From this redox reaction, liquid water is also formed [22].



To permit this phenomenon to occur, the PEMFC has the structure shown in Figure 2.2. The cell comprises a membrane electrode assembly (MEA) located between two gaskets, two bipolar plates and two current collector plates [22].

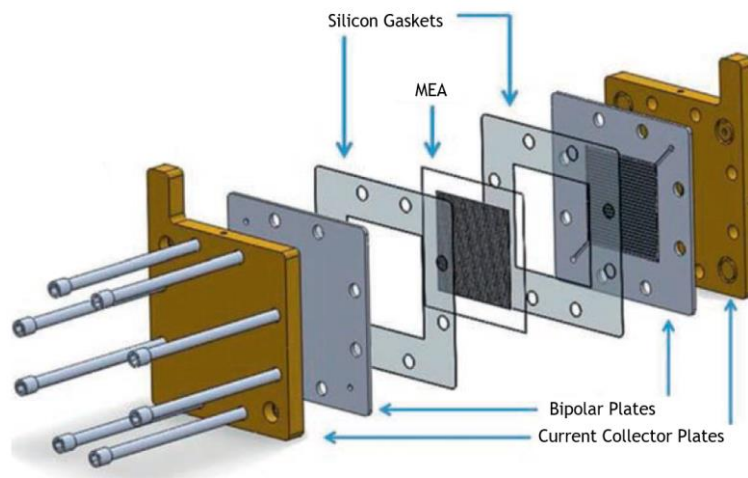


Figure 2.2. Single PEMFC structure (extracted from [22]).

2.2.1 PEMFC components

MEA

The MEA is the central piece of PEMFCs, where the electrochemical reaction (Equation (2.1)) that generates electric power takes place. It consists of a catalyst layer (CL), a gas diffusion layer (GDL), and a proton exchange membrane [22]. Figure 2.3 presents the MEA structure [24].

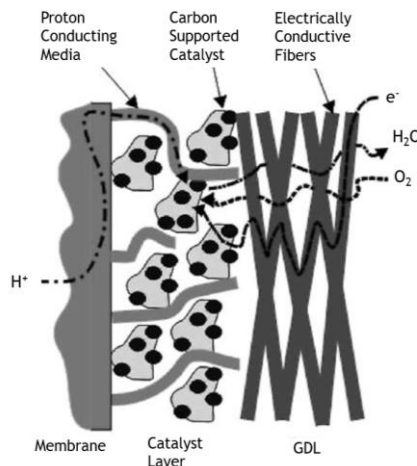


Figure 2.3. MEA structure and schematic representation of gases, protons, and electrons transport in a PEMFC (extracted from [24]).

The **membrane** is impermeable to the reaction reactants and electrons but conducts protons from the anode to the cathode. It is an electrolyte squeezed between two porous, electrically conductive electrodes [20].

The **catalyst layer** is typically made of platinum supported on carbon and is applied to the membrane (represented in Figure 2.3) or to the GDL [24]. Its main function is to accelerate the oxidation of the hydrogen on the anode (Equation (2.2)) and the reduction of oxygen on the cathode (Equation (2.3)). An ideal CL requires the minimum amount of catalyst for the reactions to happen. To do so, it is crucial to maximize the active surface area per unit of power output and to avoid obstacles to proton transport and products removal [22].



The **gas diffusion layer** allows the diffusion of the reactants to the CL and stipulates an electrical pathway for electrons and a channel for product water to go away from the electrodes [21]. It is often carbon-based and incorporates a hydrophobic material, such as polytetrafluoroethylene (PTFE). This is important to ensure the sufficient humidification of the membrane while preventing the pores of the GDL from becoming congested with water so that gases freely contact the catalyst [21, 22].

Bipolar plates and gaskets

The bipolar plates conduct the H_2 and O_2 through a channel into the MEA. The channel geometry is carefully designed to maximize the contact area between the reactant and the MEA. It is advantageous if this component exhibits chemical stability, high electrical and thermal conductivity, low contact resistance with the backing, low gas permeability, inexpensive massive production, lightweight and low volume [25]. Therefore, bipolar plates are typically made of carbon-based composite providing high corrosion resistance and lifetime. However, currently, researchers focus more on metal bipolar plates, especially for the car industry application [26].

Rubber gaskets are placed between the bipolar plate and the MEA as a sealing structure to decrease gas leakage. The performance of this component is critical for the safety and reliability of the PEMFC stacks. Thus, it is relevant to optimize the gaskets' shape and select the proper material aiming to achieve the best FC performance [27]. Silicone and fluorine caoutchouc are the typical sealing materials used in PEMFC [22].

Current collector plates

Since the membrane is not electrically conductive, the current collector plates allow a pathway for the electrons released from the hydrogen to travel from the anode to the cathode [22].

A single FC unit has a maximum potential associated. Thus, to have a higher potential is necessary to stack up several FCs in series. This is called a FC stack and it allows the cathode of one cell to be electrically connected to the anode of the following cell [20].

2.2.2 PEMFC balance of plant (BoP)

Even though the FC stack strongly influences the FC system, this component relies on the remaining support equipment, also known as BoP. Considering the fundamentals of PEMFC described, it is understandable that the BoP includes other elements such as an oxidant supply (oxygen or air), a fuel supply (hydrogen), thermal management, water management, and power units [20, 28 - 30]. An example of a PEMFC BoP is presented in Figure 2.4.

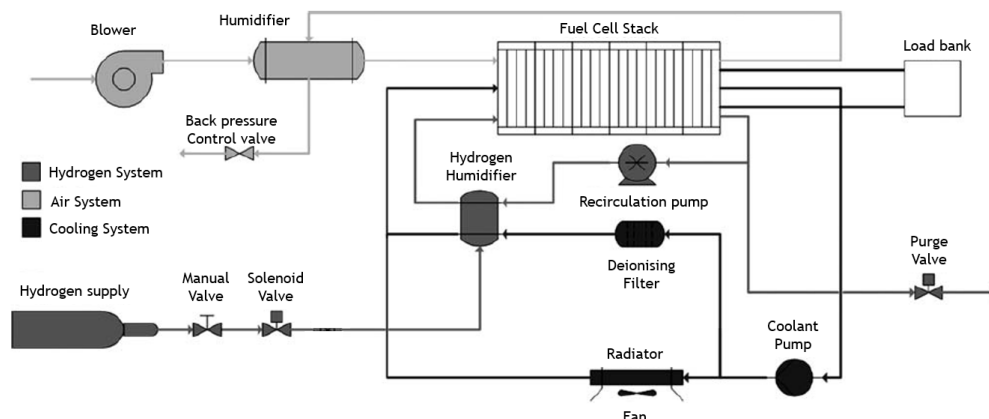


Figure 2.4. Representative example of a PEMFC BoP components: oxidant and fuel supply, and thermal and water management [29].

The air management system frequently incorporates compressors, humidifiers, heat exchangers, and flow controllers. Fuel management typically involves the same components: plus gas metering and recirculation pumps [30].

Regarding thermal management, it includes a coolant, pump, heat pipes/spread, and radiators. On the other hand, water management usually requires humidification stations, recirculation pumps, valves, and heat exchangers [28, 30].

In terms of power units, the most significant ones are AC/DC and DC/DC converters, power conditioners, controllers, and wires [30].

2.3 PEMFC thermodynamics and polarization curves

The PEMFCs are responsible for the transformation of chemical energy into electrical energy. Therefore, the thermodynamics study regarding this FC type is crucial. It enables the evaluation

of the energetic spontaneity of the reaction. Also, it allows the computation of the maximum electrical potential that can be generated from the chemical reaction (Reaction (2.1)) [31].

To calculate the maximum amount of available energy to do electrical work (W_{elec}), it is important to understand and estimate the Gibbs Free Energy (G) using Equation (2.4) [31].

$$dG = -S \cdot dT + V \cdot dP - dW_{\text{elec}} \quad (2.4)$$

This parameter G represents the exploitable energy potential, or work potential, of the system. Since FCs usually operate at constant temperature (T) and pressure (P), it is possible to assume that temperature variation (dT) and pressure variation (dP) are zero. Consequently, dG depends exclusively on dW_{elec} . The value of W_{elec} that a moving charge (Q) applies through an electrical potential difference (U) can be obtained using Equation (2.5) [31].

$$dW_{\text{elec}} = U \cdot Q \quad (2.5)$$

Assuming that Q is carried by electrons, it is calculated based on the number of moles of electrons transferred (n_{e^-}) and Faraday's constant (F) (Equation (2.6)). Therefore, the G is estimated using Equation (2.7) which results from a combination of Equations (2.4), (2.5) and (2.6) [31].

$$Q = n_{e^-} \cdot F \quad (2.6)$$

$$dG = -n_{e^-} \cdot F \cdot U \quad (2.7)$$

The hydrogen oxidation (Reaction (2.1)) under standard-state conditions (T of 298.15 K and p of 100 kPa) has dG^0 of -237 kJ and transference of 2 electrons. Also, the Faradays' constant is equal to 96 485 C mol⁻¹. Hence, the resulting standard-state reversible potential (U^0) value is equal to 1.23 V [31].

However, FCs do not operate under standard state. Thus, it is important to consider T , P and concentration variations. This can be achieved using the Nernst equation (Equation (2.8)), in which $\mathcal{R}$ is the gas constant (8.314 J mol⁻¹ K⁻¹), T is the cell temperature and $p_{\text{H}_2\text{O}}$, p_{H_2} , and p_{O_2} are the partial pressures of water, hydrogen and oxygen, respectively [31].

$$U = U^0 - \frac{\mathcal{R} \cdot T}{n_{e^-} \cdot F} \ln \left(\frac{p_{\text{H}_2\text{O}}}{p_{\text{H}_2} \cdot p_{\text{O}_2}^{1/2}} \right) \quad (2.8)$$

Even though, theoretically each FC's potential (U_{teo}) is computed through Equation (2.8), it is important to point out that, in practice the potential achieved is usually lower. The cell potential variation along current density is often represented through polarization curves, as shown in Figure 2.5 [31].

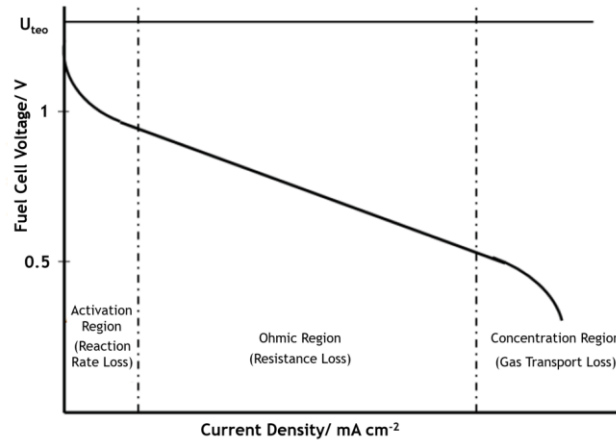


Figure 2.5. Graphical representation of the theoretical potential and real polarization curve of a PEMFC (adapted from [31]).

The gap between theoretical and real values results of irreversible losses that occur while the cell operates. Thus, the real FC's potential (U) can be computed using Equation (2.9) [31].

$$U = U^0 - \mu_{\text{act}} - \mu_{\text{ohmic}} - \mu_{\text{conc}} \quad (2.9)$$

In the first stage, these losses are activation-related and depend on the electro-catalyst material and microstructures. They represent the energy required to start and maintain the chemical reaction and occur at low current densities and high polarization values [21, 32].

The activation overpotential (μ_{act}) can be described with the Tafel equation (Equation (2.10)), where J represents the FC current density, J_E the exchange current density, and β the charge transfer coefficient [31].

$$\mu_{\text{act}} = \frac{\mathcal{R} \cdot T}{\beta \cdot n_{e^-} \cdot F} \ln\left(\frac{J}{J_E}\right) \quad (2.10)$$

While these losses do not depend proportionally on current densities, ohmic losses (μ_{ohmic}) do. This losses is caused by ionic resistance in the electrolyte and electrodes, electronic resistance in the electrodes, current collectors and interconnects, and contact resistances [21, 32].

Ohm's law can describe μ_{ohmic} as shown in Equation (2.11), where A_{FC} represents the active area, and r_{ohmic} the internal resistance which includes electric, contact, and ionic resistance [31, 32].

$$\mu_{\text{ohmic}} = J \cdot A_{FC} \cdot r_{\text{ohmic}} \quad (2.11)$$

The dependency on current density is also strong for the concentration losses (μ_{conc}) due to mass transport, and it exhibits a more substantial effect for high current densities. Also, μ_{conc} also depends on reactant activity and electrode structure [21, 32].

The value of μ_{conc} can be computed using Equation (2.12), where J_L represents the current density limit. When the FC achieves this limited current density, the reactant concentration in CL falls to zero, and the FC achieves the highest current density [31].

$$\mu_{\text{conc}} = \frac{\mathcal{R} \cdot T}{\beta \cdot n_{e^-} \cdot F} \ln \left(\frac{J_L}{J_L - J} \right) \quad (2.12)$$

After each described loss has been computed, it is possible to obtain the real cell potential through Equation (2.9).

2.4 PEMFC applications

Despite these losses, PEMFCs have received intense attention due to their wide and diverse applications. This type of FC is among the most promising electrochemical-generating devices due to their high efficiency, high power density, low emissions, and energy supply [33].

Consequently, PEMFCs have been considered for different areas such as stationaries, aeronautics, and transportation applications [30, 34].

Regarding stationary applications, PEMFC can be considered as primary power, backup power or combined heat and power [30]. Choosing PEMFCs over conventional combustion engines increases the efficiency from 30 - 40 % up to 65 %.

However, there are some drawbacks to this application, such as the high cost of grid construction and the lack of large-scale energy store infrastructure. Still, the number of stationary FC systems has been increasing worldwide. Japan, for example, plans to deploy 5.3 million ENE-FARMS devices, a fuel cell for practical homes, by 2030 [30, 35].

Recently, researchers have shown that PEMFCs exhibit properties suitable for aeronautic applications, such as emission of potential useful by-products, silent operations, solid electrolytes, and no moving parts. Moreover, the generated heat can be used for hot water and ice prevention [34].

Because of these advantages, NASA is working to discover the “21st Century” aircraft with affordable costs, safety conditions, environmental orientation, and silent operations [36].

Regarding the automotive and transportation industry, PEMFC started as a potential candidate for light-duty vehicles (LDV) due to its high-power density, high energy conversion efficiency, lightweight, and low-operating temperatures [23, 30, 37]. The latest FC LDV, Toyota Mirai, went on sale in 2020 and achieved a rating of five stars on Euro NCAP [38, 39].

However, some drawbacks prevent this application from growing. The initial high cost and the lack of widespread hydrogen refuelling stations are discouraging the cars manufacturers from investing in this technology [23, 28, 37].

Even though these disadvantages represent a limitation for LDV, they are manageable for heavy-duty vehicles (HDV). It happens since they already have high investment costs, and their route can be planned considering the existing refuelling stops [28].

Moreover, the application of FC in HDV has recently raised enough attention as HDVs are responsible for a significant part of global CO₂ emissions. In the United States HDVs represent around 23 % of the total carbon dioxide emissions [28].

PEMFCs can easily help with the emissions' reduction. Still, the different drive cycles, operating conditions, and longer lifetimes result in a substantial improvement in durability and a greater focus on fuel efficiency compared with LDVs [28].

2.5 FC drive cycles

Helpful input information for the emissions and fuel consumption studies includes the drive cycle. It consists of speed and elevation values evolution over time or distance. When the drive cycle is plotted as speed over time, it is easier to use it and directly compute the power demand, the FASTSim drive cycles are usually displayed that way. On the other hand, when it is plotted as speed-distance, such as VECTO ones, the power demand estimation requires middle calculations.

These cycles are especially valuable when they are representative of how a vehicle will operate in a target application. For instance, heavy-duty cycles are different from light-duty cycles, as well as European cycles have some distinctions from ones in USA. However, evaluating if the cycle is representative can be challenging [40, 41].

The driving cycle characterization is a crucial step in the mechanical energy or power demand evaluation for different cycles [41-43].

This comparison between distinct driving cycles can be accomplished computing the kinetic parameters: characteristic acceleration ($\tilde{a}$), positive kinetic energy (PKE), aerodynamic speed (v_{aero}) and kinetic intensity (ki) [41-43].

The $\tilde{a}$ parameter indicates the inertial work to accelerate or raise the vehicle per mass unit and per distance unit over the cycle. It represents the positive part of kinetic and potential energy per distance associated with moving a vehicle over a drive cycle (Equation (2.13)) [41].

$$\tilde{a} = \frac{\sum_{j=1}^{N-1} \left[\frac{1}{2} (v_{j+1}^2 - v_j^2) + g(l_{j+1} - l_j) \right]}{D_{cycle}} \quad (2.13)$$

Here the v represents the vehicle velocity, l is the height, and D_{cycle} is the distance of the cycle. For a constant height, and linear speed increase, the characteristic acceleration equals the actual acceleration value [41].

The $\tilde{a}$ and K_{PKE} parameters have a proportional progression [41]. K_{PKE} values reveal how smooth or aggressive the driving is regarding the speed variations. It also implies vehicle-to-vehicle interaction on the road and can be computed using Equation (2.14) [42].

$$K_{PKE} = \frac{\sum_{j=1}^{N-1} |v_{j+1}^2 - v_j^2|}{D_{\text{cycle}}} \quad (2.14)$$

The aerodynamic speed is linked to the impact of the aerodynamics on vehicle fuel usage. It can be computed using Equation (2.15), where t represents the time [41].

$$v_{\text{aero}} = \sqrt{\frac{\sum_{j=1}^{N-1} \left(\frac{v_{j+1}^3 + v_{j+1}^2 \cdot v_j + v_{j+1} \cdot v_j^2 + v_j^3}{4} \right) (t_{j+1} - t_j)}{D_{\text{cycle}}}} \quad (2.15)$$

For a constant speed, the aerodynamic speed equals the speed of the cycle [41].

The combination of $\tilde{a}$ and v_{aero} results in the kinetics intensity, which provides a ratio of energy used to accelerate over the energy used to overcome drag. This parameter can be estimated using Equation (2.16) [41].

$$k_i = \frac{\tilde{a}}{v_{\text{aero}}} \quad (2.16)$$

As the $\tilde{a}$ increases or v_{aero} decreases, k_i increases, resulting in a driving with more aggressive accelerations and lower average speeds [41].

The key factor about these parameters is that they characterize the speed and height variations over the time of a given driving cycle regardless of the vehicle specifications. That is the reason why they are useful when comparing different cycles [41].

2.6 Computation of the power demand of the PEMFC

The information provided by a drive cycle, together with the vehicle properties, allows the computation of the mechanical power demand. To do so, it is important to first understand which resistance forces affect a moving vehicle (Figure 2.6). Then, knowing the power results from the multiplication of the force and the speed, it is possible to understand that the total mechanical power demand ($\dot{W}_{\text{mech}}$) comprises the power to overcome the inertia ($\dot{W}_{\text{inertia}}$), the rolling resistance ($\dot{W}_{\text{rol}}$), the gravitational potential ($\dot{W}_{\text{climb}}$), and the aerodynamic drag ($\dot{W}_{\text{air}}$) (Equation (2.17)) [11, 41].

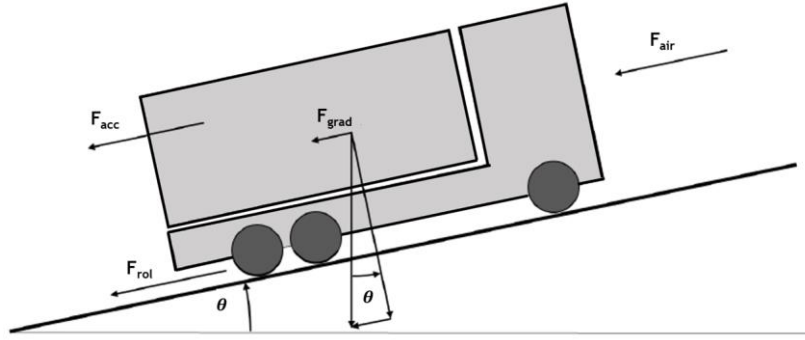


Figure 2.6. Representation of the forces that affect a vehicle moving to the right (adapted from [41]).

$$\dot{W}_{mech} = \dot{W}_{inertia} + \dot{W}_{climb} + \dot{W}_{rol} + \dot{W}_{drag} \quad (2.17)$$

Here $\dot{W}_{inertia}$ is the power required to overcome the gravitational acceleration resistance and accelerate a vehicle. The translational acceleration of the vehicle and the acceleration of the rotary masses, like tires and electric motors, are considered by the rotational inertia factor (e) in Equation (2.18), where m_{empty} represents the truck empty mass, $m_{payload}$ the payload mass, v the vehicle velocity, and a the acceleration [11].

$$\dot{W}_{inertia} = (e \cdot m_{empty} + m_{payload}) \cdot a \cdot v \quad (2.18)$$

The $\dot{W}_{climb}$ is the resistance increase when driving uphill and decrease when driving downhill (estimated using Equation (2.19)). The pitch angle of the hillside (θ) is often zero in standard drive cycles [11, 41].

$$\dot{W}_{climb} = (m_{empty} + m_{payload}) \cdot g \cdot \sin(\theta) \cdot v \quad (2.19)$$

The $\dot{W}_{rol}$ is the resistance resulting from the friction between road and tires and the deformation work of the tires. The rolling resistance power can be approximated as Equation (2.20), where C_R represents the rolling resistance coefficient [11, 41].

$$\dot{W}_{rol} = C_R \cdot (m_{empty} + m_{payload}) \cdot g \cdot \cos(\theta) \cdot v \quad (2.20)$$

The $\dot{W}_{drag}$ is the resistance characterized by the drag coefficient (C_D) that quantifies the drag of the truck and depends on the density of the air (ρ_{air}), the vehicle's cross-sectional area ($A_{vehicle}$), and the speed, as shown in Equation (2.21) [11, 41].

$$\dot{W}_{drag} = \frac{1}{2} \cdot \rho_{air} \cdot C_D \cdot A_{vehicle} \cdot v^3 \quad (2.21)$$

$\dot{W}_{climb}$ can be positive or negative depending on whether there is an increase or decrease in height and speed. Thus, the power can be produced ($\dot{W}_{kinetic}$) or required ($\dot{W}_{NET}$), they can be computed through Equations (2.22), and (2.23).

$$\dot{W}_{NET} = \sum \text{positive}(\dot{W}_{\text{mech}}) \quad (2.22)$$

$$\dot{W}_{\text{kinetic}} = \sum \text{negative}(\dot{W}_{\text{mech}}) \quad (2.23)$$

Even though the $\dot{W}_{NET}$ is the power required for the vehicle motion estimated using Equations (2.17) and (2.22), in a real scenario, it is important to consider the energy dissipation in the system. Here, it is possible to see that the FC power demand computation must consider the powertrain (ε_{PT}), the converters, the battery or capacitor, and the FC efficiencies.

Thus, the NET power demand from the hybrid system ($\dot{W}_{NET,d}$) can be computed using Equation (2.24) [44].

$$\dot{W}_{NET,d} = \frac{\dot{W}_{NET}}{\varepsilon_{PT}} \quad (2.24)$$

2.7 Existing simulators

Nowadays, there are several useful simulators designed to analyze the power demand of a vehicle to complete a drive cycle as “FASTSim”. This simulator is supported by the U.S. Department of Vehicle Technologies Office. This is a vehicle powertrain analysis tool that provides a simple approach to comparing powertrains and estimating the impact of technological improvement on light- and heavy-duty vehicle efficiency. Several different types of fuel storage, fuel converter, motor, traction battery, wheel, and energy management strategy can be simulated [15, 16].

A similar existing program is called VECTO, which is a great tool to simulate HDVs combustion engines and estimate the energy demand, fuel consumption, and CO₂ emissions. This tool has been developed by the European Commission, aiming to reflect the European fleet [17].

These are two strong tools in heavy-duty vehicle simulation. Still, a tool more oriented to the hydrogen vehicles analysis is needed to satisfy the market needs. In this regard, this paper describes and uses a new simulator developed by DLR that allows the power demand estimation of a specified heavy-duty vehicle and the evaluation of the most suitable hybrid (hydrogen-electric) strategy for the energy supply.

2.8 PEMFC in hybrid systems

The FC systems (Figure 2.3) operate together with a battery or capacitor in a hybrid system, increasing the FC lifetime. During acceleration, the battery/capacitor and the FC stacks jointly handle power peaks. During breaking, part of the energy generated allows the battery to

charge. During cruising, the FC stacks satisfy the main power demand and charge the battery simultaneously [45].

The PEMFC stack works as the primary energy supplier and the battery/capacitor works as the auxiliary. To avoid the potential discrepancy between the energy sources, a DC/DC converter is used to equalize the potential level, while a DC/AC is used to invert the current to feed the motor. An example of the fundamental structure of this strategy is represented in Figure 2.7 [46].

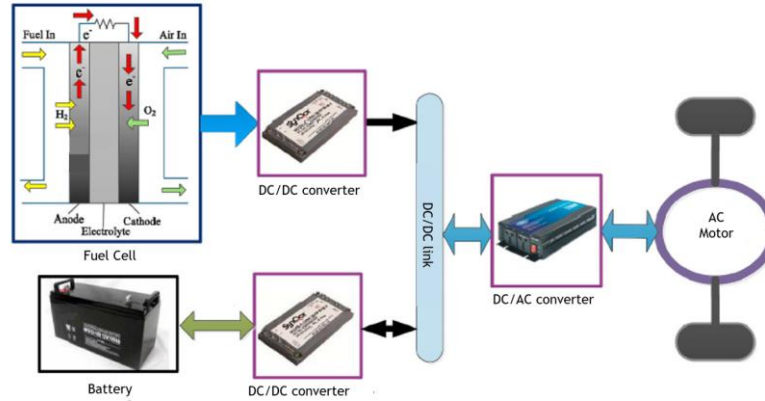


Figure 2.7. The basic structure of a PEMFC and battery hybrid system for vehicles application (adapted from [45]).

Different strategies for the hybrid system can be implemented. However, this is the most preferred one in research since it has great flexibility in controlling the power flow for both the FC and the battery systems [45].

2.9 Hybrid system topology

The $\dot{W}_{mech}$ that a heavy-duty vehicle requires to complete the desired drive cycle is sometimes accomplished using a fuel cell stack only. However, sometimes the energy that the FC produces is not enough, and a hybrid system can be advantageous. In hybrid systems, the main power supply is the FC, and a battery or capacitor is added as an auxiliary supply.

This strategy can be used to allow the FC to operate in optimum conditions, soften the change of the FC operation conditions, and provide an extra power peak during short periods. Consequently, it leads to increased efficiency and a reduction of FC degradation conditions resulting in a lifetime extension.

The mechanical power demand in the electric motor ($\dot{W}_{NET}$ and $\dot{W}_{kinetic}$) can be converted in current mechanical demand (i) assuming a constant potential supply to the electrical motor (U) through Equation (2.25).

$$i = \frac{\dot{W}}{U} \quad (2.25)$$

The mechanical current demand can be split into the FC mechanical current demand ($i_{FC,HV}$) and the battery/capacitor mechanical current demand ($i_{Bat,HV}$), as the shown in Figure 2.8 .

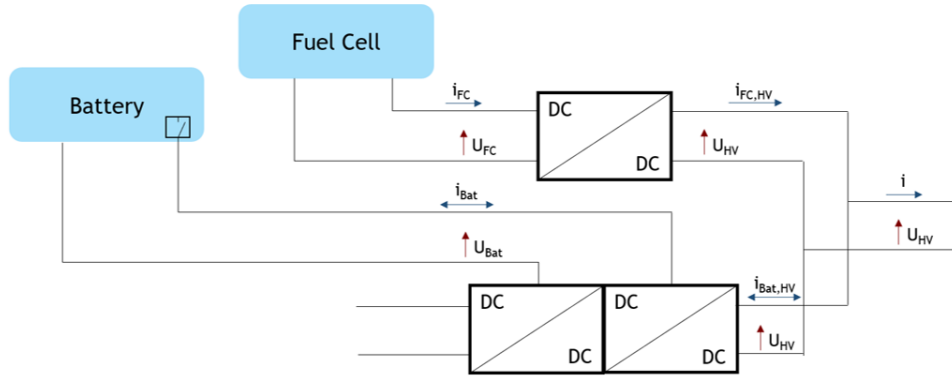


Figure 2.8. Fuel cell and battery hybrid system and current and potential distribution.

The DC/DC converter device is used to change the potential level of the electric power output. When the device converts a low potential current (LV) into higher potential current (HV). This is the boost mode operation. The system operates in buck mode when the device transforms a high potential current into a lower potential current. The operations are in Figure 2.9.

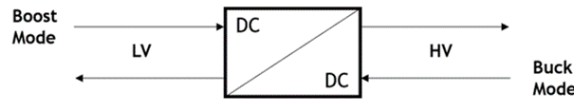


Figure 2.9. DC/DC converter device operation modes.

In boost mode, the relationship between current the low potential current (i_{LV}) and high potential current (i_{HV}) can be translated by Equation (2.26), where $\varepsilon_{DC/DC}$ represents the converter efficiency, U_{HV} represents the high potential value, and U_{LV} represents the low potential value.

$$\varepsilon_{DC/DC} \cdot U_{LV} \cdot i_{LV} = U_{HV} \cdot i_{HV} \quad (2.26)$$

Regarding the Buck mode, this relation is transformed in Equation (2.27).

$$U_{LV} \cdot i_{LV} = \varepsilon_{DC/DC} \cdot U_{HV} \cdot i_{HV} \quad (2.27)$$

As seen in Figure 2.8, the FC DC/DC converter operates exclusively in boost mode, representing that the current is drained from the system (positive i values). On the other hand, the battery DC/DC converter can operate in boost mode when the battery discharges and in buck mode when it charges.

3 Modelling and computer implementation

The phenomenological model and simulator were developed for analyzing the energy demand of heavy-duty vehicles equipped with a hybrid power system of a FC / LiB units. It works similar to FASTSim and VECTO but it is oriented for HDV with hybrid FC / LiB technology.

Furthermore, the focus of this simulator is to compute the power demand from the FC system, and from the stack itself. This information can be further used to develop accelerated stress tests for stacks and stacks components representing real life operations. To do so, several driving cycles available from FASTSim, DriveCAT, and VECTO were used to estimate the driving power required to fulfil the cycle. The data obtained was relevant in estimating the power demand from the FC with a simple hybridization strategy and all the FC's operating conditions (heat rejection, gas flows efficiencies, among others).

3.1 Simulator model structure

The core of the simulator was developed in Python with spyder. One short example is presented in Appendix A -. Its logic structure can be divided into two distinct stages, as shown schematically in Figure 3.1. The first is the “mechanical simulation”, which computes the power demand of the vehicle. The second one is the “power splitting simulation”, which computes the power fraction required from the FC and the fraction required from the LiB.

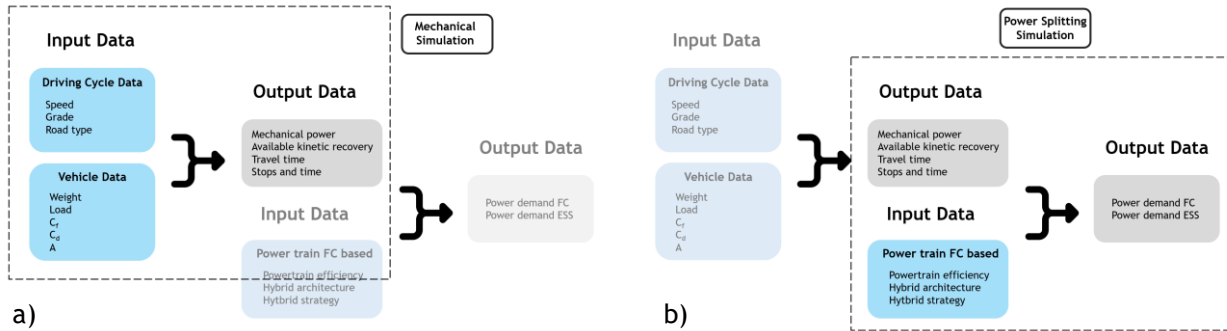


Figure 3.1. Representative scheme of the simulator logic structure: a) is the first stage - “mechanical simulation” and b) is the second stage - “power splitting simulation”.

3.1.1 Mechanical simulation

The mechanical simulation can be defined in three steps: the drive cycle definition, the vehicle definition, and the mechanical power demand computation. The first step is to select the drive cycle from the listed options presented in Chapter 4.1. This represents the mission profile that the user aims to be accomplished by a vehicle. Once the drive cycle is selected, the simulator plots the velocity and grade vs time and computes the kinetic parameters using Equations

(2.13), (2.14), (2.15), and (2.16). Characteristic acceleration, positive kinetic energy, aerodynamic speed, and kinetic intensity are the parameters considered for this simulator.

With a drive cycle defined, the simulator starts the following step. Here, the user specifies the vehicle properties presented in Appendix A -. If the user does not identify some property, the simulator assumes the default values, which are representative of an HDV (Appendix A -).

Knowing the drive cycle and the vehicle properties, the simulator starts the final step - the mechanical power demand computation using Equation (2.17). Additionally, the power demand is distinguished between $\dot{W}_{kinetic}$ and $\dot{W}_{NET}$ through Equations (2.22) and (2.23). Lastly, the $\dot{W}_{NET,d}$ is computed using Equation (2.24).

In order to display the net energy demand ($W_{NET,d}$) and the recoverable energy ($W_{kinetic}$), the power is converted into energy through Equations (3.1) and (3.2).

$$W_{NET,d} = \int \dot{W}_{NET,d}(t) dt \quad (3.1)$$

$$W_{kinetic} = \int \dot{W}_{kinetic}(t) dt \quad (3.2)$$

With this output, the simulator plots $\dot{W}_{NET,d}$ and $\dot{W}_{kinetic}$ evolution over time and the respective drive cycle with the slope variation (grade), as shown in Figure 3.2. A histogram with the fraction of time spent in each power range like the one presented in Figure 3.3 is also displayed.

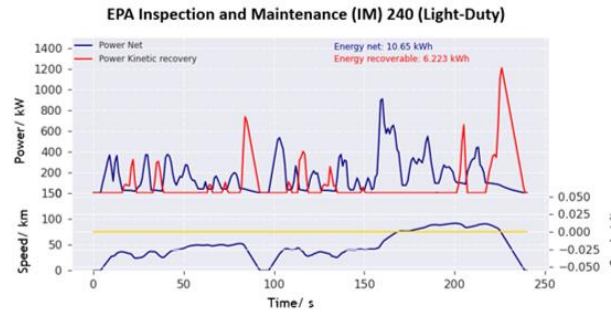


Figure 3.2. $W_{NET,d}$ and $W_{kinetic}$ evolution over time, and respective drive cycle.

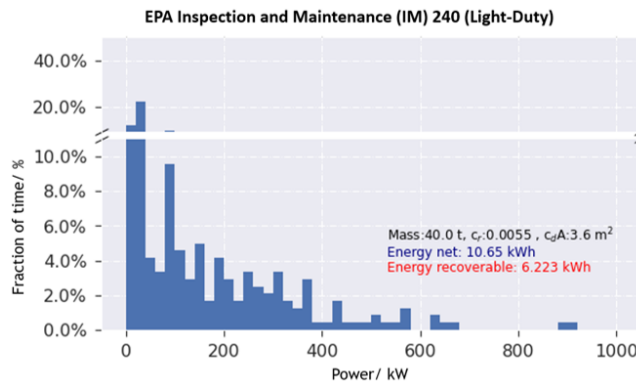


Figure 3.3. Histogram with the drive cycle time fraction spent in each power range.

3.1.2 Power splitting simulation

Once the power demand has been computed during the mechanical simulation, the power splitting simulation begins. In this second stage, the simulator computes the energy required from each energy supplier used in the hybrid system, like the one displayed in Figure 2.8. Thus, there are three steps like the first stage: the definition of the FC specification, the battery/capacitor definition, and the computation of the power demand of each device.

Regarding the FC, they are categorized into three groups: the FC's operating conditions, the polarization curve, and the cathode properties. For the first category, the parameters to be defined are the FC's active surface area (A_{FC}) and the number of FCs stacked (NC).

The polarization curve parameters include the FC's resistivity per surface area (R_{FC}) and the potential and current density reference point values (U_0 and J_0). These values can be defined by the user, or the simulator assumes the default value for the R_{FC} ($4 \times 10^{-6} \Omega \text{ m}^2$) and J_0 ($10\,000 \text{ A m}^{-2}$). The user can also define the cathode pressure (P_{cathode}). Otherwise, the simulator considers the default value of $1.5 \times 10^5 \text{ Pa}$.

Additionally, the battery specifications can be set by the user, or the simulator assumes the default values presented in Table 3.1.

Table 3.1. Battery input parameters and respective default values.

Battery's properties	Default Value
Battery's capacity/ A s	93 600
Battery's resistance/ Ω	15×10^{-5}
Battery's minimum stage of charge (-)	0.12
Battery's maximum stage of charge (-)	0.98

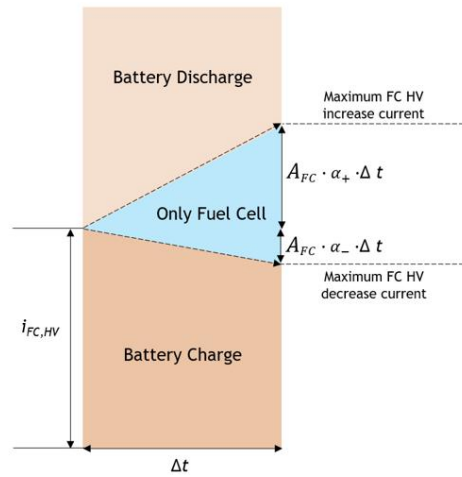
Other than the battery and FC properties, the converter efficiency ($\varepsilon_{DC/DC}$), and the BoP components, such as the air compressor's isentropic efficiency (η_{comp}), and the radiator's heat rejection capacity (QDT_{kpi}) must be defined. Otherwise, the simulator considers $\varepsilon_{DC/DC}$ equal to 0.92, the QDT_{kpi} as $1\,450 \text{ W K}^{-1}$ and estimates the η_{comp} through an interpolation function.

Lastly, regarding the hybrid strategy system, there are several different strategies. The one defined in this simulator is to limit the current demand increase and decreasing the FC. Thus, three parameters can be defined by the user, which are the maximum current increase and decrease per time unit (α_+ , and α_-) and the constant potential on the high potential side (U_{HV}). If the user does not define these parameters, the simulator considers the default values presented in Table 3.2.

Table 3.2. Hybrid system strategy input parameters and respective default values.

Hybrid strategy parameters	Default Value
$\alpha_+ / \text{A m}^{-2} \text{s}^{-1}$	242
$\alpha_- / \text{A m}^{-2} \text{s}^{-1}$	162
U_{HV} / V	800

The calculations are centred on the power split approach presented in Figure 3.4 [47], [48]. There are two situations possible to be distinguished: the power demand increasing and the power demand decreasing. In both situations the kinetic recovery (W_{kinetic}) is not considered. The load increasing in the FC is limited to a certain current increase per time unit (α_+). On the other hand, the load decrease in the FC is limited to a certain current decrease per time unit (α_-). These two parameters can be adjusted depending on the fuel cell performance and the desired stability in the fuel cell power output.


 Figure 3.4. Power splitting approach used in the simulator to compute the $i_{Bat,HV}$, and $i_{FC,HV}$.

Power demand increase

The power demand increase results in an increment of the fuel inflow and the reagents consumption. When the power demand increases faster than the fuel supply, the FC starts to operate in starvation conditions resulting in its degradation. To avoid this situation, the current density produced by the FC during a certain period (Δt) increases until a certain limit (α_+). This limit must be wisely defined as an input. If the user does not define it, the simulator assumes a default value of $242 \text{ A cm}^{-2} \text{s}^{-1}$.

After an increment in the power demand, the simulator computes the new FC operating point. To do that, the first step is to use Equation (3.3) and compute the maximum current in the low

potential side of the DC/DC converter ($i_{FC,max}$), knowing the previous current value ($i_{FC,n}$), as displayed in Figure 2.8 and Figure 2.9 [47], [48].

$$i_{FC,max} = i_{FC,n} + A_{FC} \cdot \alpha_+ \cdot \Delta t \quad (3.3)$$

Knowing $i_{FC,max}$, the maximum current demand at the high potential side ($i_{FC,HV,max}$) can be estimated using Equation (2.26).

Comparing the current demand (i) with $i_{FC,HV,max}$, two situations can occur. If $i < i_{FC,HV,max}$, the fuel cell can handle the power increase and the $i_{FC,HV}$ is defined as equal to i , which is computed using Equation (2.25) considering a constant potential (U_{HV}) and $\dot{W}$ equal to $\dot{W}_{NET}$. If $i \geq i_{FC,HV,max}$, the fuel cell current ($i_{FC,HV}$) is set to the $i_{FC,HV,max}$ value and the i_{FC} is computed using Equation (2.26), where U_{FC} is estimated using the polarization curve. In this simulator, the polarization curve (at 80 °C) is approximated by Equation (3.4) [47], [48]. The U_0 parameter was computed using Equation (3.5) to force the polarization curve of a single FC to go through the potential value of 0.65 V when the current density is 1 A cm⁻² [49].

$$U_{FC} = N_C \cdot \left[U_0 - 0.07 \cdot \log_{10} \left(\frac{i_{FC}/A_{FC}}{J_0} \right) - R_{FC} \cdot \frac{i_{FC}}{A_{FC}} \right] \quad (3.4)$$

$$U_0 = 0.650 + R_{FC} \cdot J_0 \quad (3.5)$$

The polarization curves of a single FC and a FC stack are presented in Figure 3.5.

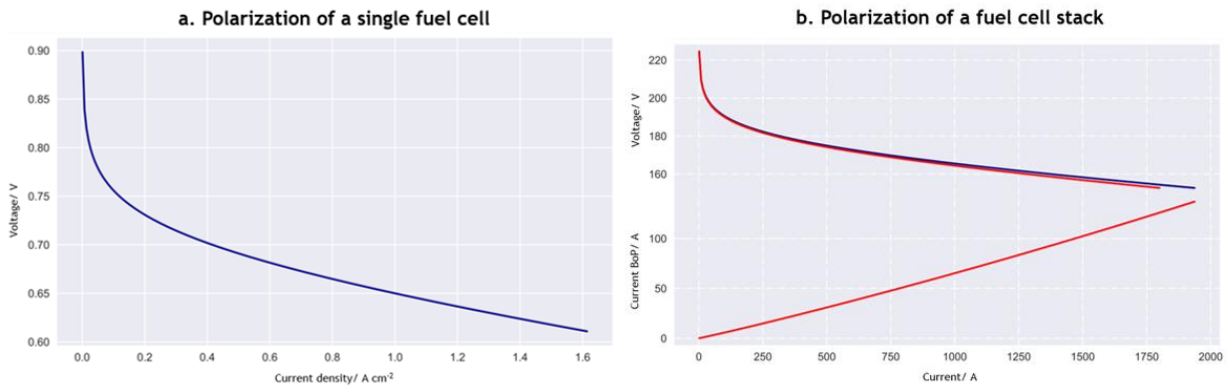


Figure 3.5. Polarization curves for a single FC and a FC stack.

On the other hand, the battery current ($i_{Bat,HV}$) is the balance current demand (Equation (3.6)) and i_{Bat} is estimated using Equation (2.26). The U_{Bat} is computed using Equation (3.7), where $U_{Bat,n}$ is the previous potential, and r_{Bat} is the battery resistance.

$$i_{Bat,HV} = i - i_{FC,HV} \quad (3.6)$$

$$U_{\text{Bat}} = U_{\text{Bat},n} - r_{\text{Bat}} \cdot i_{\text{Bat}} \quad (3.7)$$

This procedure is graphically explained in Figure 3.6, from a certain current $i_{FC,HV}$ three possible regions are accessible: battery discharges (point 1), FC operates exclusively (points 2 and 3), and battery charges (point 4). The point 1 describes the situation where $i \geq i_{FC,HV,max}$, and the point 2 describes the $i < i_{FC,HV,max}$ situation.

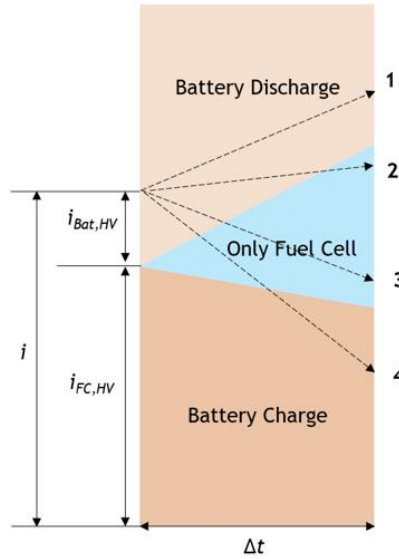


Figure 3.6. Representation of the three possible changes in current demand: battery discharge (point 1), FC operates exclusively (points 2 and 3), and battery charges (point 4).

Power demand decrease

To avoid all the power decrease settling on the fuel cell, the current excess is used to recharge the battery. The current density produced by the FC during a certain period (Δt) decreases until limit (α_-) that must be wisely defined as an input. If the user does not define it, the simulator assumes a default value of $100 \text{ A cm}^{-2} \text{ s}^{-1}$.

In a similar way to the power demand increase situation, the simulator computes the new FC operation point. Thus, it starts by estimating the maximum current decrease ($i_{FC,min}$) using Equation (3.8). Once the $i_{FC,min}$ is known, $i_{FC,HV,min}$ can be computed with Equation (2.26).

$$i_{FC,min} = i_{FC,n} - A_{FC} \cdot \alpha_- \cdot \Delta t \quad (3.8)$$

Comparing the current demand (i) with $i_{FC,HV,min}$, two situations can occur. If $i \geq i_{FC,HV,min}$, the fuel cell can handle the power decrease and the $i_{FC,HV}$ is defined as equal to i , which is computed using Equation (2.25) considering a constant potential (U_{HV}) and $\dot{W}$ equal to $\dot{W}_{NET}$.

If $i < i_{FC,HV,min}$, the fuel cell current ($i_{FC,HV}$) is set to $i_{FC,HV,min}$ value, and the i_{FC} is computed using Equation (2.26), where U_{FC} is also a function of i_{FC} (Equation (3.4)). This situation is represented graphically as point 3 in Figure 3.6.

On the other hand, as the battery is charging, the DC/DC converter operates in buck mode, so the current $I_{Bat,HV}$ is the remaining current demand (Equation (3.6)) and i_{Bat} is estimated using Equation (2.27), where the U_{Bat} is also a function of i_{Bat} (Equation (3.7)). As this is a charging situation, the i_{Bat} is a negative value. This situation is represented graphically through the point 4 in Figure 3.6.

The battery unit acts as the auxiliary supplier. However, it is important to point out that the battery current output depends on its state of charge (SoC). Thus, there is a requirement to evaluate if the battery has enough energy storage to provide power during a certain time. The new SoC ($S_{SoC,n+1}$) can be estimated through Equation (3.9), knowing the previous SoC ($S_{SoC,n}$). The capacity of the battery (C_{Bat}) is defined by the user.

$$S_{SoC,n+1} = S_{SoC,n} - \frac{i_{Bat} \cdot C_{Bat}}{dt} \quad (3.9)$$

The maximum current that the battery can release ($i_{dis,max}$) during a certain period (Δt) can be computed through Equation (3.10), where $S_{SoC,min}$ represents the minimum SoC for the battery and is defined by the user.

$$i_{dis,max} = \frac{(S_{SoC,n+1} - S_{SoC,min}) \cdot C_{Bat}}{dt} \quad (3.10)$$

The simulator considers that $i_{dis,max}$ is never exceeded to avoid damaging conditions or sudden power drops. When the total current produced from the hybrid system is lower than the current demand, the simulator assumes that the demand is not fulfilled, and both the FC and battery operates at their maximum.

The maximum current that the battery can absorb during a certain period of time ($i_{char,max}$) is computed using Equation (3.11), where $S_{SoC,max}$ represents the maximum SoC for the battery and is defined by the user.

$$i_{char,max} = \frac{(S_{SoC,n+1} - S_{SoC,max}) \cdot C_{Bat}}{dt} \quad (3.11)$$

The simulator considers that $i_{char,max}$ is never exceeded to avoid damaging conditions or sudden power drops. When the current decreases and exceeds the $i_{char,max}$, the simulator assumes that the battery absorbs the $i_{char,max}$, and the FC operates at $i_{FC,HV,min}$.

Based on the estimated i_{Bat} value, the simulator computes $\dot{W}_{Bat}$ using Equation (2.25) and the energy demand using Equation (3.12).

$$W_{\text{Bat}} = \int \dot{W}_{\text{Bat}}(t) dt \quad (3.12)$$

Regarding the FC, the simulator computes the current produced by the FC that is used for power production ($i_{FC,NET}$) using Equation (3.13), where $i_{FC,Bruto}$ represents the total current demand, which includes the $i_{FC,NET}$ and the current needed for the BoP ($i_{FC,BoP}$).

$$i_{FC,NET} = i_{FC,Bruto} - i_{FC,BoP} \quad (3.13)$$

The $i_{FC,BoP}$ includes the current demand for pumping the H₂ supply, the coolant, and the air compressor ($i_{FC,comp}$). In this simulator, the H₂ and coolant pumping requirements are estimated to correspond to 10 % of the $i_{FC,comp}$ (Equation (3.14)).

$$i_{FC,BoP} = 1.1 \cdot i_{FC,comp} \quad (3.14)$$

To compute $i_{FC,comp}$, the simulator starts estimating the number of O₂ moles consumed at the cathode ($\dot{n}_{O_2,cathode}$) using Equation (3.15), as explained in Appendix C -.

$$\dot{n}_{O_2,cathode} = NC \cdot \frac{i_{FC,Bruto}}{4 \cdot F} \quad (3.15)$$

Subsequently, the air mass consumption rate ($\dot{m}_{air,cathode}$) is estimated with Equation (3.16), where $\chi_{O_2,air}$ is the O₂ molar fraction in the air and is equal to 0.21, and the $M_{O_2,cathode}$ is the O₂ mass molar which is 32 g mol⁻¹.

$$\dot{m}_{air,cathode} = \frac{M_{O_2,cathode} \cdot \dot{n}_{O_2,cathode}}{\chi_{O_2,air}} \quad (3.16)$$

Knowing $\dot{n}_{O_2,cathode}$, the simulator computes the power demand for the compressor ($\dot{W}_{FC,comp}$) through Equation (3.17). The specific heat capacity of the air ($C_{p,air}$) was set as 1 006 J kg⁻¹ K⁻¹, and the gas was considered as ideal with a heat capacity ratio ($\gamma_{cathode}$) of 1.4. The $P_{cathode}$ is the pressure of the flow going out of the compressor and getting in the cathode which is defined by the user. The $P_{in,comp}$, and $T_{in,comp}$ are respectively the pressure and temperature of the air getting in the compressor, which are equal to and 10⁵ Pa and 353.15 K. The temperature of the air getting in the compressor is set as the operating temperature of the FC (T_{rated}). Using Equation (2.25) the $i_{FC,comp}$ can be estimated as well as $i_{FC,NET}$ (Equation (3.13)).

$$\dot{W}_{FC,comp} = \frac{C_{p,air} \cdot T_{rated}}{\eta_{comp}} \cdot \left[\left(\frac{P_{cathode}}{P_{in,comp}} \right)^{\frac{\gamma_{cathode}-1}{\gamma_{cathode}}} - 1 \right] \cdot \dot{m}_{air,cathode} \quad (3.17)$$

The thermodynamic equation is further explained in Appendix D -.

The simulator iteratively attributes values to $i_{FC,Bruto}$, compute $i_{FC,NET}$ and compare it with the i_{FC} until similar values are obtained - minimizing $|i_{FC,NET} - i_{FC}|$.

Additionally, the hydrogen flowrate demand and the coolant consumption rate and the heat exchanger conditions are also computed. To do so, the hydrogen consumption rate ($\dot{n}_{H_2,anode}$) is estimated using Equation (3.18) (explanations are presented in Appendix C -).

$$\dot{n}_{H_2,anode} = N_C \cdot \frac{i_{FC,Bruto}}{2 \cdot F} \quad (3.18)$$

On the other hand, to evaluate the coolant consumption rate and the heat exchanger conditions it is important to understand the scheme in Figure 3.7.

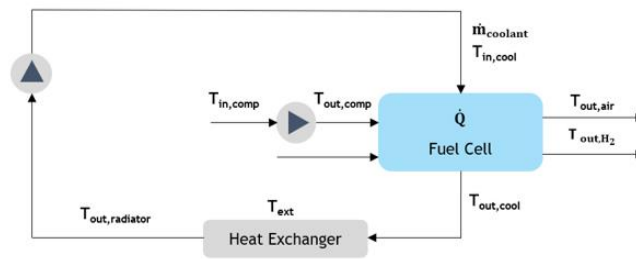


Figure 3.7. Fuel cell thermal management schematic representation.

The FC has some heat losses ($\dot{Q}_{FC}$) that are higher for higher current values as shown in Figure 2.5. $\dot{Q}_{FC}$ can be computed using Equation (3.19), where ε_{FC} is the efficiency of the FC computed using the Equation (3.20) and $\dot{W}_{FC}$ is the power demand of the FC, which can be estimated using Equation (2.25) (assuming i as $i_{FC,Bruto}$ and U as U_{FC}). The simulator considers that ε_{FC} includes the different electrochemical efficiencies.

$$\dot{Q}_{FC} = \frac{\dot{W}_{FC}}{\varepsilon_{FC}} \quad (3.19)$$

$$\varepsilon_{FC} = \frac{U_{FC}}{1.253} \quad (3.20)$$

This heat loss results in the FC's temperature increase, so the coolant needs to increase for stabilizing temperature of the FC. From thermodynamic and using Equation (3.21), the coolant mass flowrate ($\dot{m}_{coolant}$) can be estimated. The $C_{p,coolant}$ is the specific heat capacity of the coolant ($3500 \text{ J kg}^{-1} \text{ K}^{-1}$), and the ΔT_{stack} is the temperature variation of the coolant ($T_{out,cool} - T_{in,cool}$), which the simulator assumes a default of 12 K. In ideal conditions, the temperature of the flow of coolant going out of the FC ($T_{out,cool}$) should be similar to the temperature of the H_2 and air flows going out of the FC ($T_{out,H_2}, T_{out,air}$) and to the operating temperature of the FC (T_{rated}) [31].

$$\dot{Q}_{FC} = \dot{m}_{coolant} \cdot C_{p,coolant} \cdot \Delta T_{stack} \quad (3.21)$$

Regarding the heat exchanger, the simulator can evaluate two different situations. A heat rejection capacity can be defined by the user ($\dot{Q}_{QDT,kpi}$), or the desired flow temperature going out of the FC and going in the radiator ($T_{out,cool}$) can be defined. On the first situation, the simulator computes the temperature difference between the coolant out flow ($T_{out,cool}$) and the environment (T_{ext}). This difference (ΔT_{max}) is estimated through Equation (3.22).

$$\Delta T_{max} = \frac{\dot{Q}_{FC}}{\dot{Q}_{QDT,kpi}} \quad (3.22)$$

Considering a worst-case scenario where T_{ext} is 313.15 K, the $T_{out,cool}$ can be computed. The resulting value represents the $T_{min,rated}$, which is the FC's stack operating temperature that allows the max heat power dissipation. Otherwise, the $T_{out,cool}$ can be defined as T_{rated} (353.15 K), and the ΔT_{max} estimated. Then, the heat rejection capacity ($\dot{Q}_{QDT,computed}$) needed to achieve that temperature variation can be computed through Equation (3.23) [47], [48].

$$\dot{Q}_{QDT,computed} = \frac{\dot{Q}_{FC}}{(T_{rated} - T_{ext})} \quad (3.23)$$

3.2 User interface

Even though the simulator comprises a strong tool to allow the hybrid strategy evaluation, it is important to make it user-friendly, so users that are not familiar with programming can still take advantage of this tool. Therefore, a user interface was developed.

This was written in Python Jupyter Notebook, using the core of the calculations present in the simulator together with explanations and input boxes. This interface is required to easily perform some test studies to optimize the vehicle components such as the fuel cell and battery.

Some images of this interface and explanations are presented and discussed in Appendix E -.

4 Results and discussion

The purpose of this simulator in this project was the study and characterization of the FC power demand in FC / LiB vehicles, particularly heavy-duty vehicles. Thus, it was important to find a drive cycle and vehicle that were representative of the European operation. After that, it was possible to evaluate the outcome of the simulator by simulating an example. The influence of the hybrid strategy on power demand was also studied in this section.

4.1 Comparison of drive cycles and vehicles

A drive cycle or vehicle can be considered typical when they are close to real-case scenarios. To find the most typical cycles from the list presented in Chapter 1, it was important to do some comparison tests between different cycles. Moreover, the understanding of the influence of each property of the vehicle on the power demand was a crucial point as well.

Firstly, four US cycles and three EU cycles were selected to be tested. This selection was based on a primary analysis and elimination of the cycles with high acceleration phases, meaning fast increments in speed, high-speed values (over 100 km h^{-1}), and frequent speed changes, like the example shown in Figure 4.1.

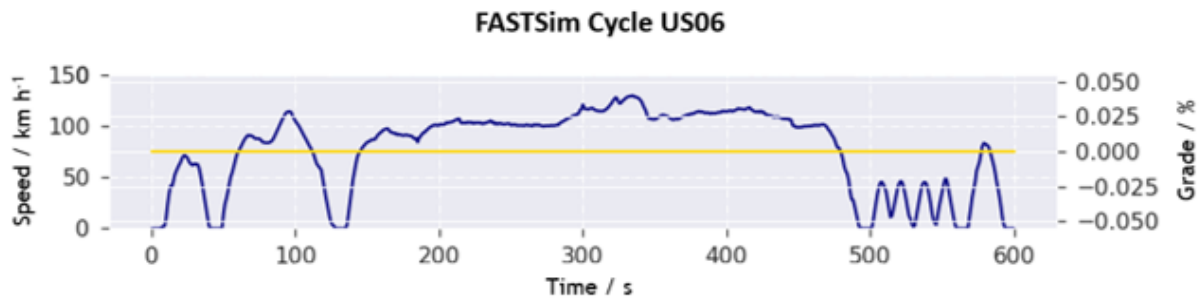


Figure 4.1. Drive cycle representative of light-duty vehicles: speed (blue) and grade (yellow) evolution along time.

These were eliminatory factors since they are suited for light-duty vehicles, so heavier vehicles would demand extremely high-power values. In fact, heavy-duty vehicles exhibit more stable speeds, slower accelerations, and lower speed values.

According to this logical thinking, four cycles from US institutions were chosen. Three cycles were selected from DriveCAT: the “California Air Resources Board Heavy Heavy-Duty Diesel Truck” (HHDDT), the “NREL Port Drayage Composite Cycle” (California), and the “Urban Dynamometer Driving Schedule for Heavy-Duty Vehicles” (UDDS HD). Only one cycle was selected from FASTSim: the “Long Haul Drive Cycle” (LHDC). They are exhibited in Figure 4.2.

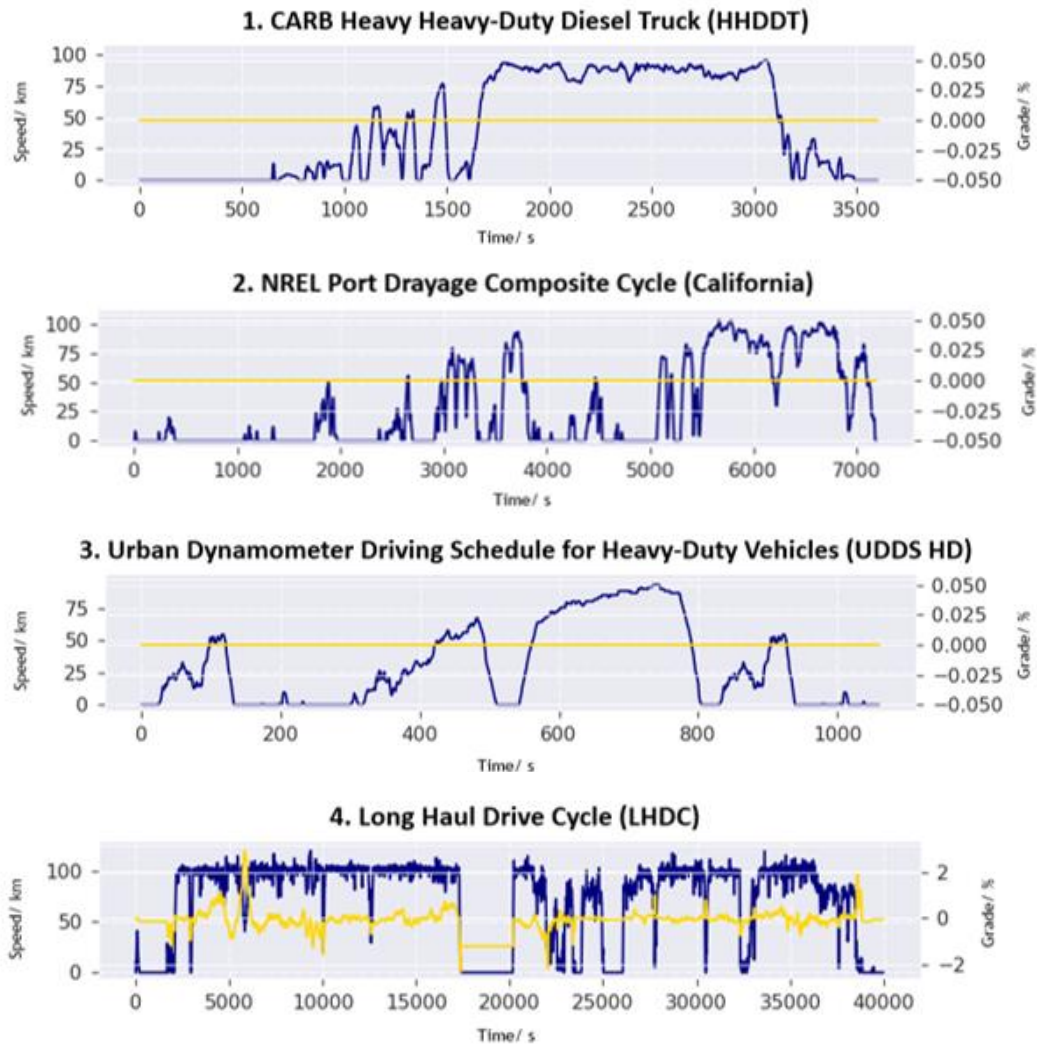


Figure 4.2. US drive cycles representative of heavy-duty vehicles: HHDDT, California, UDDS HD, and LHDC. Representation of speed (blue) and grade (yellow) evolution along time.

The HHDDT is a cycle that represents a heavy-duty commercial truck operation. It was developed by the California Air Resources Board with West Virginia University, and four segments can be identified. It starts with a 10-minute idle segment, followed by a creep moment lasting for 4 minutes, which is typically a slow operation instant or waiting in a queue at a port. After that, the transient moment occurs for 11 minutes, which is typical of near-port driving. The cycle ends with a high-cruise segment lasting for 35 minutes [50]. This cycle lasts approximately 1 hour total, so it is representative of short transportations, for example between two different cities.

The California cycle was developed by the NREL, a national laboratory of the U.S. Department of Energy. To construct this cycle, the researchers gathered data from 30 Class 8 drayage trucks operating at the Port of Long Beach and Los Angeles. After that, they used the clustering methodology to organize the data and the drive cycle generation portion of DRIVE to generate the cycle [51].

The California cycle is a combination of 4 segments or clusters. The first cluster lasts for 20 minutes and represents trips with long waiting in queue periods and short durations of driving followed by long stationary idle time. The second cluster has a duration of about 20 minutes as well and represents the near dock driving, with segments of extended idle and medium-speed driving components. The third one also lasts for the same time and is representative of local higher speed and shorter trips. The longest cluster is the final one, with approximately 50 minutes and is typical of longer, higher-speed trips on metropolitan area highways [51].

The UDDS HD was developed by the Economic Partnership Agreement and was specially designed for heavy-duty vehicles. This cycle is typical of transient driving and lasts approximately 18 minutes [51]-[66].

The LHDC cycle is also representative of heavy-duty cycles and lasts for over 11 hours, which represents a working day [67]-[69]. Even though this is the only measured cycle considering the grade variation resulting from climbing periods, it exhibits speed values over the heavy-duty vehicles' typical maximum speed of 100 km h^{-1} . Still, it is evident that the speed peaks over this value do not occur with a significant consistency, and it is possible to exclude those peaks by truncating the cycle speed to a reasonable point.

This method of truncation has been used by DLR in studies of the power demands of FC. This is chosen over rescaling to preserve the cycle behaviour regarding the slopes of the power increases and decreases.

The kinetic parameters of each US cycle were computed by the simulator, and the output is exhibited in Table 4.1. The average speed in time is the average speed excluding stopped moments.

Table 4.1. Kinetic parameters computed by the simulator for the US selected cycles: HHDDT, California, UDDS HD, and LHDC.

Kinetic Parameter	HHDDT	California	UDDS HD	LHDC
$\tilde{a} / \text{m s}^{-2}$	0.0535	0.0921	0.1366	0.0574
$K_{PKE} / \text{m s}^{-2}$	0.1070	0.1842	0.2732	0.1110
$v_{\text{aero}} / \text{m s}^{-1}$	22.67	21.55	19.01	26.70
k_i / km^{-1}	0.1041	0.1982	0.3781	0.0805
Time/ min	60	120	18	667
Distance/ km	41.92	56.67	8.94	803.03
Maximum Speed/ km h^{-1}	95.43	103.27	93.34	120.53
Average Speed in time/ km h^{-1}	52.97	42.25	33.88	70.64

The analysis of Table 4.1 shows that HHDDT and LHDC are the cycles with lower values of $\tilde{a}$, K_{PKE} , and k_i , which translates a less aggressive driving, with soft accelerations, and more stable speed values. On the other hand, the UDDS HD reveals aggressive driving, which is not typical of heavy-duty vehicles. The soft driving is important to avoid FC degradation.

The HHDDT and LHDC cycles also have higher values of average speeds, resulting in higher v_{aero} related to highway road driving. This information can be confirmed in Figure 4.2, where it is clear that both cycles represent a high-speed cycle, while the California and UDDS HD cycles represent transient driving.

To compute the power demand, it was required to set the vehicle specifications first. For that reason, vehicle specifications were collected from numerous previous research, as explained in Appendix A -. Considering those specifications of the vehicle, the power demand over time for each drive cycle was plotted in Figure 4.3.

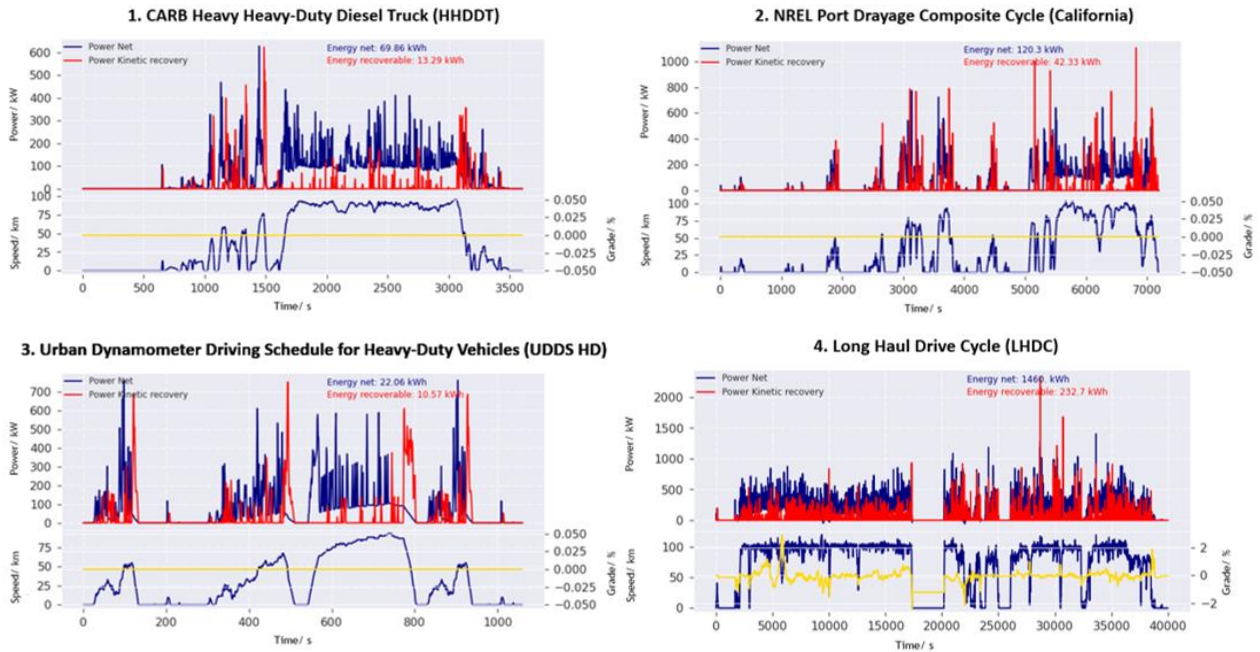


Figure 4.3. Power demand distinguished in power net and power kinetic recovery and respective evolution over time for the selected US drive cycles.

The visible plots show that the LHDC has significantly higher energy demand values (1 460 kW h). Also, this cycle exhibits a wider range of power, which makes it harder to apply the FC as the power source. The power peaks demand present in every cycle can also be aggressive for the FC operation. However, it is possible to overcome this using a LiB or capacitor.

As the cycles have different time durations, instead of comparing the total energy demand is more reasonable to compare the total average power demand of each cycle. The values of the net power (N_p) demand during acceleration and the recoverable power (R_p) produced during deceleration are presented in Table 4.2. The LHDC cycle has the highest N_p value (131.40 kW),

while the California one has the lowest (60.19 kW). On the other hand, the R_p produced is the highest for the UDDS HD (35.89 kW) and the lowest for the HHDDT (13.27 kW).

Table 4.2. Average net power demand and recoverable power produced for each selected US cycle.

Cycle	N_p / kW	R_p / kW
HHDDT	69.78	13.27
California	60.19	21.18
UDDS HD	74.91	35.89
LHDC	131.40	20.94

In order to choose the most typical cycle, there is another significant plot to compare: the fraction of time spent in each power range. It is presented for each cycle in Figure 4.4.

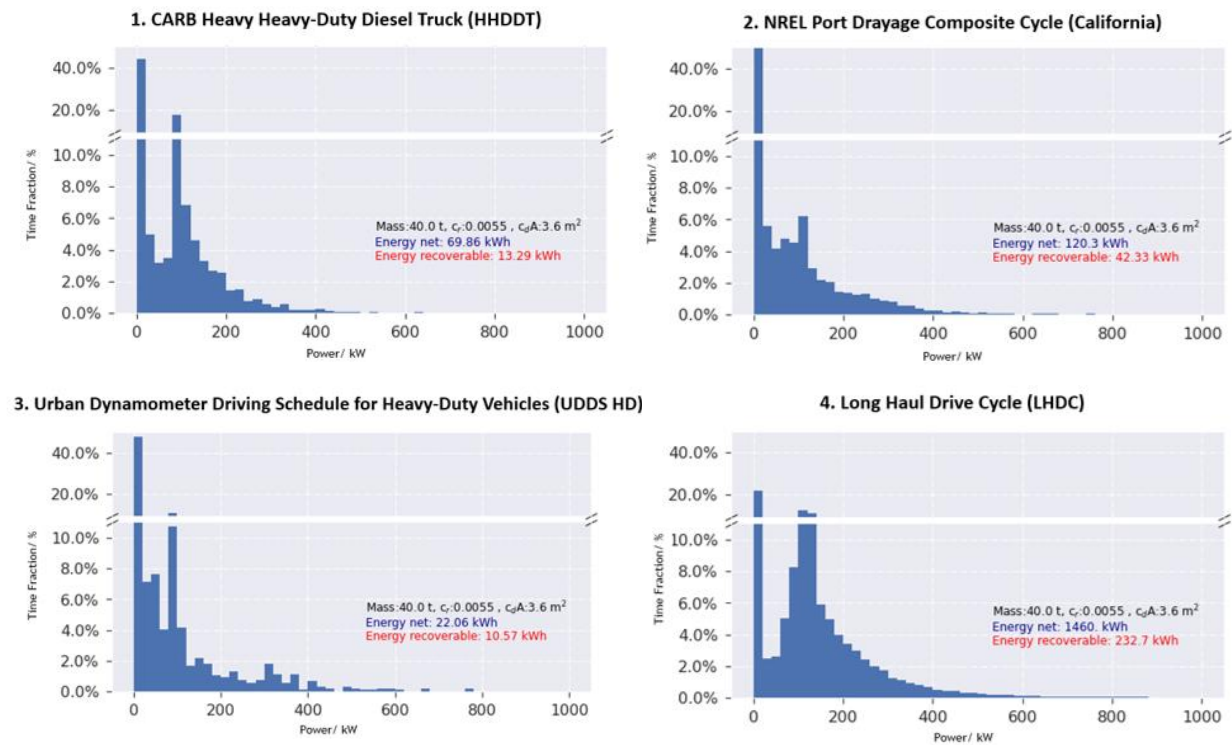


Figure 4.4. Histogram with the drive cycle time fraction spent in each power range for the four selected US cycles.

This analysis allows the understanding of the type of road driven since it is possible to observe if most of the time is spent in higher or lower power demand. In the cases under observation, a clear distinction is visible. The HHDDT and LHDC cycles exhibit a higher fraction of the time spent in high power demand values, typical of highway driving, while the UDDS HD shows a higher fraction of the time spent in lower power demand. On the other hand, the California

cycle has a more homogeneous distribution of the time spent over the different power ranges. Additionally, this is the cycle with the highest time spent for null values of power demand.

After gathering this information, it was possible to find which cycle is the most representative of US heavy-duty vehicles. Even though the LHDC is the only one that considers the altitude variation, this cycle exhibits high-speed values and power demands. On the other hand, the kinetic parameters of UDDS HD translate aggressive driving, so it is not the most suitable cycle.

The two remaining cycles are representative of different types of driving, and once the highway is more representative of heavy-duty vehicles, the HHDDT cycle was the selected one.

A similar analysis was done on three European drive cycles selected from VECTO: “Long Haul Cycle” (LH), “Urban Cycle” (urban), and “Regional Delivery Cycle” (RD). However, the VECTO cycles are given in terms of equi-spaced speed vs distance, as mentioned in Chapter 2.5. Thus, middle calculations were required to obtain equi-spaced speed vs time, as presented in Figure 4.5. Still, this strategy may generate artificial peak accelerations.

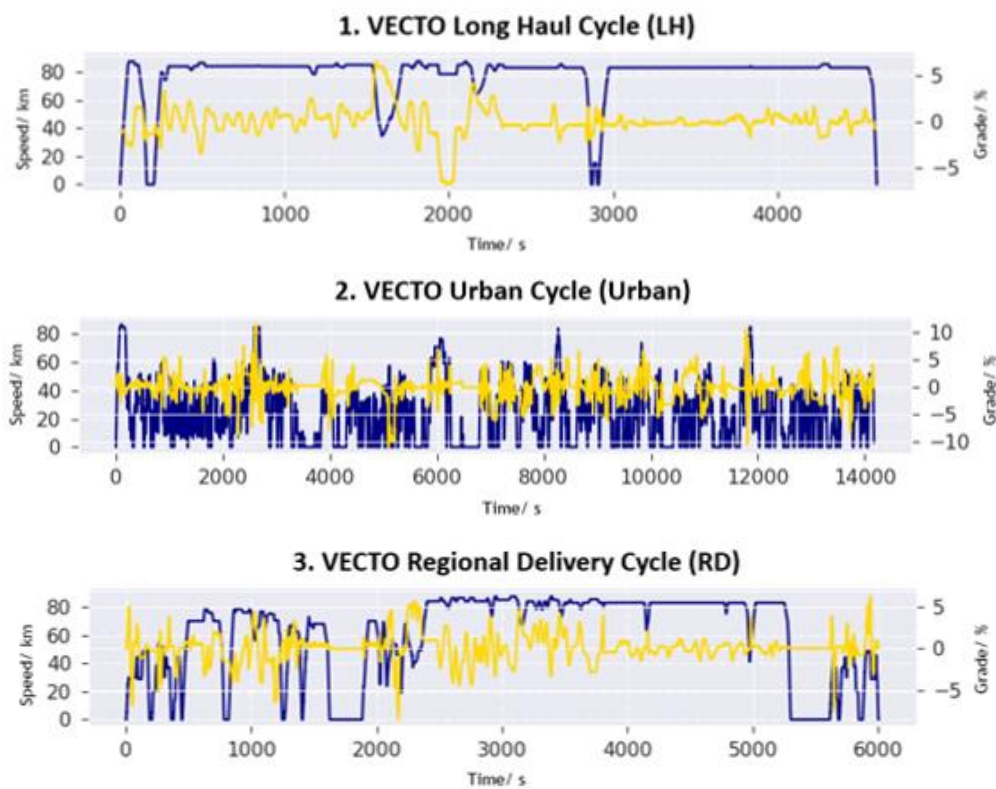


Figure 4.5. US drive cycles representative of heavy-duty vehicles: LH, urban, and RD. Representation of the speed (blue) and grade (yellow) evolution along time.

The LH is a heavy-duty driving cycle that lasts for 77 minutes with maximum speeds of 87.5 km h^{-1} . This is a cycle from VECTO and represents a constant speed cycle with some stops, which can be representative of deliveries between different cities.

The urban cycle is also from VECTO and lasts for 236 minutes with a maximum speed of 86.93. Still, this is not a good example of heavy-duty cycles since the speed changes too often and aggressively.

The third VECTO cycle (RD cycle) has a duration of 100 minutes and a maximum speed of 87.5 km h⁻¹. In the RD cycle is possible to identify the different segments in a similar way as in the HHDDT cycle. The creep moment lasts for the first 8 minutes, followed by the transient moment, which occurs for 30 minutes, and the last segment represents the high-cruise segment.

The kinetic parameters of each cycle are presented in Table 4.3.

Table 4.3. Kinetic parameters computed by the simulator for the EU selected cycles: LH, urban, and RD.

Kinetic Parameter	LH	urban	RD
$\ddot{a} / \text{m s}^{-2}$	0.0516	0.1967	0.0811
$K_{PKE} / \text{m s}^{-2}$	0.0309	0.3381	0.0744
$v_{\text{aero}} / \text{m s}^{-1}$	22.77	12.86	21.15
k_i / km^{-1}	0.0995	1.1888	0.1814
Time/ min	77	236	100
Distance/ km	100.19	100.03	100.00
Maximum Speed/ km h ⁻¹	87.50	86.93	87.50
Average Speed in time/ km h ⁻¹	80.01	28.39	66.51

Analyzing Table 4.3 is clear that the urban cycle is the one exhibiting higher values of $\ddot{a}$, K_{PKE} , and k_i , which translates an aggressive driving, regular and intense acceleration, and unstable speed. On the other hand, the LH and RD have low values of these parameters, representing a cycle more typical of heavy-duty vehicles. Also, these two cycles show high values of v_{aero} , resulting in higher average speeds related to highway road driving. This information can be confirmed in Figure 4.5, where it is clear that both cycles represent a high-speed cycle, while the urban cycle represents transient driving.

In a similar way to the US cycles, the power demand considering the default values described in Appendix A - was computed and the simulator output graphs are exhibited in Figure 4.6.

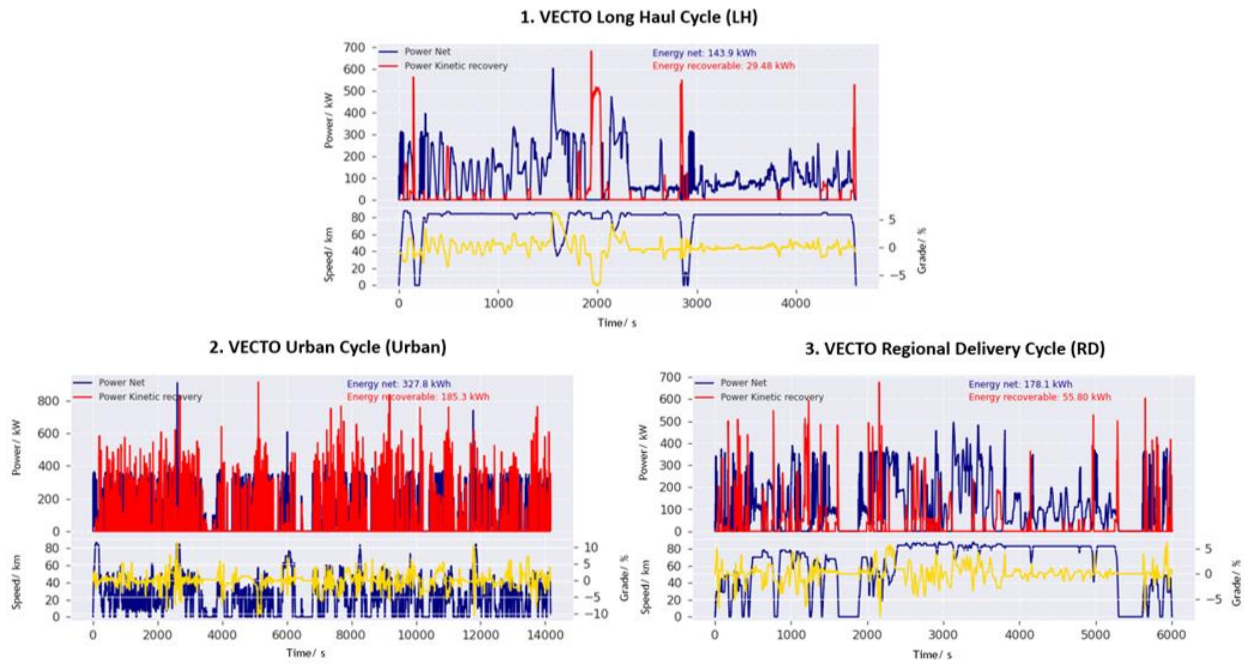


Figure 4.6. Representation of the power demand distinguished in power net and power kinetic recovery and respective evolution over time for the selected EU drive cycles.

The urban power demand plot exhibit extremely fast power variations, which makes it harder to apply the FC as the power source since it can be aggressive for the FC operation.

As the cycles have different time durations, is more reasonable to compare the total average power demand of each cycle instead of comparing the total energy demand. The N_p and R_p values were computed and are presented in Table 4.4. The LH cycle has the highest N_p value (112.48 kW), while the urban one has the lowest (83.24 kW). On the other hand, the R_p produced is the highest for the urban (47.04 kW) and the lowest for the LH (23.05 kW).

Table 4.4. Average net power demand (N_p) and recoverable power produced (R_p) for each selected EU cycle.

Cycle	N_p / kW	R_p / kW
LH	112.48	23.05
Urban	83.24	47.04
RD	106.73	33.43

The time spent in each power range for the three different EU cycles is graphically represented in Figure 4.7.

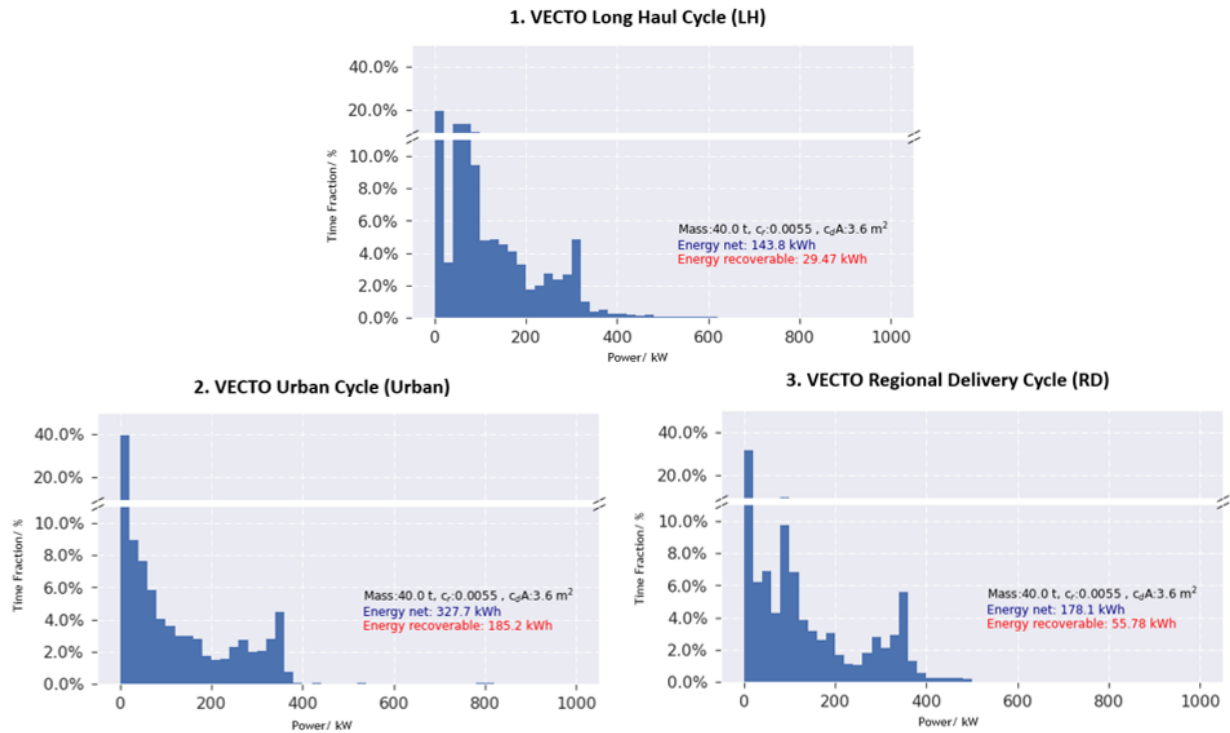


Figure 4.7. Histogram with the drive cycle time fraction spent in each power range for the three selected EU cycles.

This comparison showed that the LH and RD cycles are more suited for heavy-duty vehicles. As the different driving segments are easily distinguished in the RD, this is the best one to represent the EU heavy-duty vehicles.

Comparing the kinetic parameters of the US and EU cycles (Table 4.1 and Table 4.3), it is possible to see similarities between the cycles. Still, the RD cycle exhibits a vaguely higher $\tilde{a}$ value which is understandable since it is the only one that considers the height variation. Additionally, the US cycle is slightly more aggressive due to higher values of K_{PKE} .

Following the decision on which cycle to use, the effect of the properties of the vehicle on the power demand was studied. Each parameter value, presented in Appendix A -, was increased and decreased by a factor (Δd) for the EU and US representative cycles. The vehicle properties variation influence on the power demand is discussed in Appendix F -.

The evolution of the net energy (N_E) and recoverable energy (R_E) variation over the property variation for the RD cycle is presented in Figure 4.8.

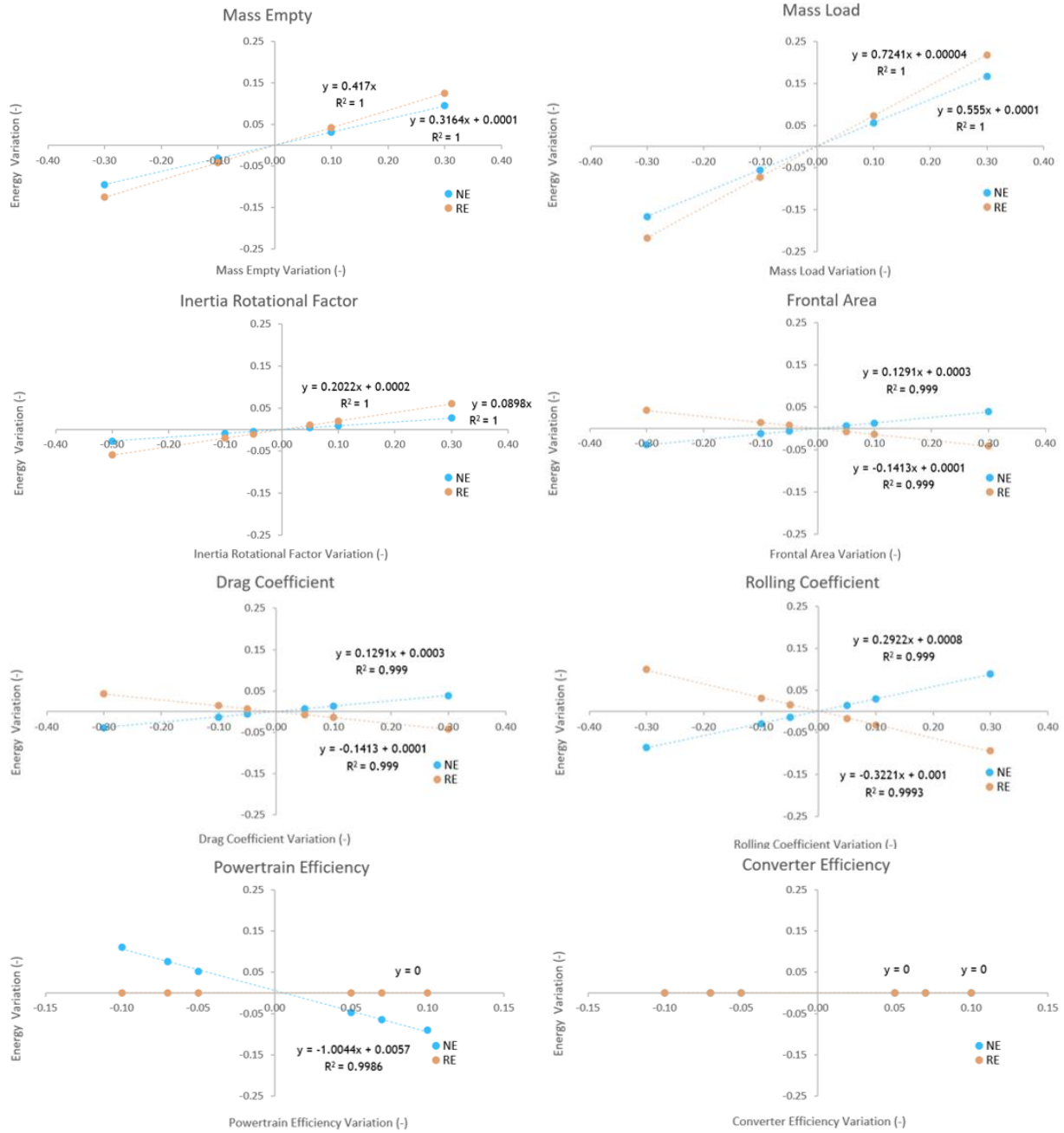


Figure 4.8. The N_E and R_E variation along each vehicle property variation aiming the analysis of the vehicle properties' effect on power demand considering the EU cycle (RD).

Analyzing the first two plots, it is possible to see that an increment in the vehicle mass results in an increase in both N_E and R_E . Still, the mass load exhibits a stronger influence since a variation on this parameter (Δd) of 10 % results in a power demand increase of almost double when compared with the Δd of the mass empty.

The e exhibits a more significant influence in the R_E than in the N_E . Still, both N_E and R_E increase when increasing the e .

The C_D and A_{vehicle} influences were also analyzed, and it was possible to see that both have a similar effect on the power demand, as expected from Equation (2.21). The increment in these properties result in higher N_E and lower R_E values. The same occurs for the C_R .

The increment on the powertrain efficiency results in the N_E decrease only, and a variation on the converter efficiency does not influence N_E and R_E .

From a global point of view, the N_E is more influenced by the powertrain efficiency and the mass load. Regarding the R_E , the mass load and the e have the strongest influence.

The influence of each vehicle property depends also on the drive cycle. To understand the influence of each cycle parameter in the relation between the energy demand and the vehicle property, the evolution along each cycle parameter value was evaluated as shown in Appendix G -. Six cycles were tested: HHDDT, California, UDDS HV, LHDC, LH, and RD.

The relationship between the energy demand and both the mass empty and the mass load ($\Delta W/\Delta m_{\text{empty}}$ and $\Delta W/\Delta m_{\text{payload}}$ respectively) exhibited similar variations. As Figure 4.9 shows, for the mass empty, neither K_{PKE} nor the $\tilde{a}$ values influence this relationship, while the v_{aero} and k_i do.

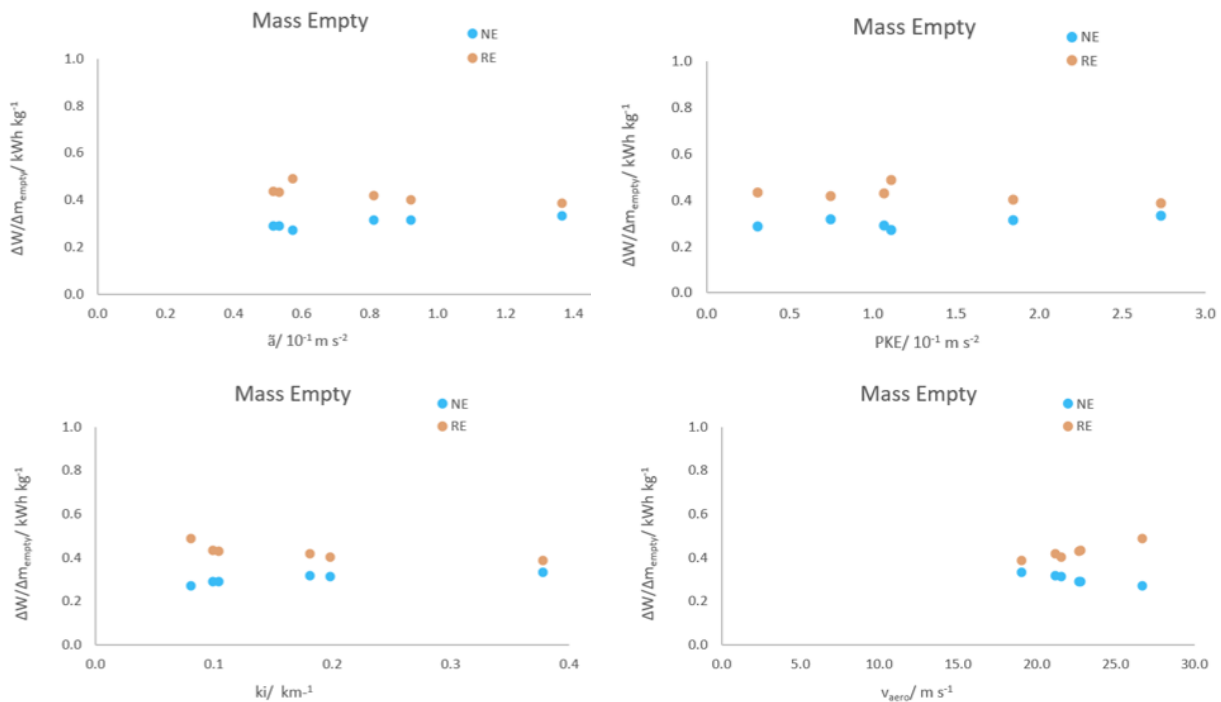


Figure 4.9. Graphical representation of the relation between the energy variation and the mass empty ($\Delta W/\Delta m_{\text{empty}}$) for different values of the cycle parameters: K_{PKE} , $\tilde{a}$, v_{aero} , and k_i .

Low values of k_i and high values of v_{aero} result in an intensification of the influence of the mass variation on the R_E . On the other hand, the opposite occurs with the influence of the mass variation on the N_E .

In a similar way to the mass empty and mass load, the relationship between the energy variation and both the frontal area and drag and rolling coefficients ($\Delta W/\Delta A_{\text{vehicle}}$, $\Delta W/\Delta C_D$, and $\Delta W/\Delta C_R$ respectively) are alike. The representation regarding A_{vehicle} is displayed in Figure 4.10.

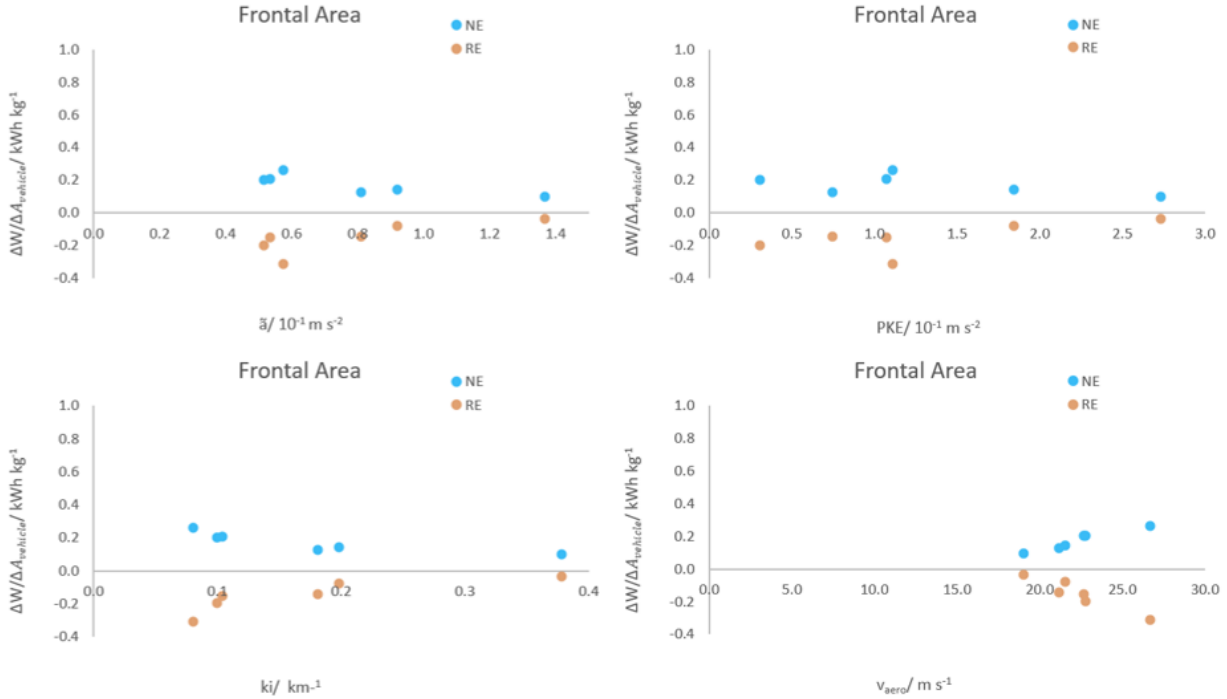


Figure 4.10. Graphical representation of the relation between the energy variation and the vehicle frontal area ($\Delta W/\Delta A_{\text{vehicle}}$) for different values of the cycle parameters: K_{PKE} , $\tilde{a}$, v_{aero} , and k_i .

The plot analysis shows that cycles with different K_{PKE} or $\tilde{a}$ do not affect significantly the $\Delta W/\Delta A_{\text{vehicle}}$ values, while high v_{aero} values and low k_i values result in an intensification of the N_E sensitivity to the A_{vehicle} , C_D , and C_R variations.

Comparing the different results, it is possible to understand that the v_{aero} is the cycle kinetic parameter with the highest influence on the energy demand sensitivity to each vehicle property variation.

Considering the technologies that are likely to be further developed and introduced in around 5 to 8 years, accordingly to the International Council on Clean Transportation (icct) a reduction of 27 % in C_D , 23 % in C_R and 1 000 kg in m_{empty} can be achieved [70]. For the European cycle (RD), these reductions result in an increment of 8.7 % on the R_E and a decrease of 12.0 % on the N_E . These values were obtained using the developed simulator.

4.2 A representative example

After the evaluation of the properties of the drive cycle and vehicle, the developed simulator was used to compute the total power demand and the SoC of the battery. To analyze the simulator output, the parameters used were the ones defined in Appendix H -. Under the established conditions, the plot exhibited in Figure 4.11 was obtained using the simulator.

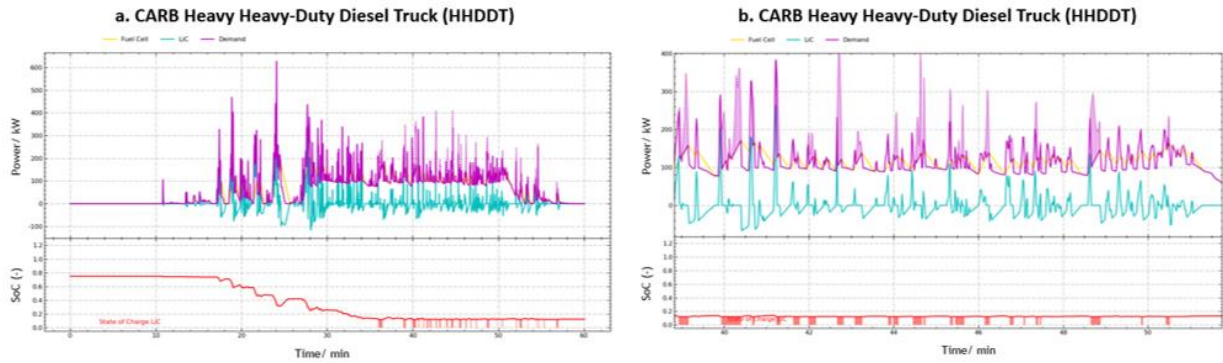


Figure 4.11. Power demand or produced and battery's SoC evolution over time for the HHDDT cycle, for an entire drive cycle and for a limited period.

On the plot on the left, it is visible that the battery shows some periods where the SoC is at the minimum value allowed. This means that there might be some moments where the FC-battery system cannot deliver the power required by the vehicle since the battery has no current to provide. A closer look at these periods (plot on the right) indicates that at the same time as the SoC reaches its minimum value, the power demand represented by the dotted purple line is sometimes above the power produced represented by the purple line.

Consequently, the vehicle does not achieve the target speed of the drive cycle. It is possible to deduce that the battery capacity is not enough to work with the defined FC.

Other than the SoC and power evolution over time, the developed simulator also computes the FC's current density and potential evolution, and it is displayed and described in Appendix I -.

Regarding the power splitting, the two plots presented in Figure 4.12 represent another output of the simulator. It is possible to see some differences in the power distribution of the FC and LiB. The FC exhibits positive values only, while the LiB can have positive and negative values. The negative values represent the periods when the power demand decreases and the energy surplus is absorbed by the LiB.

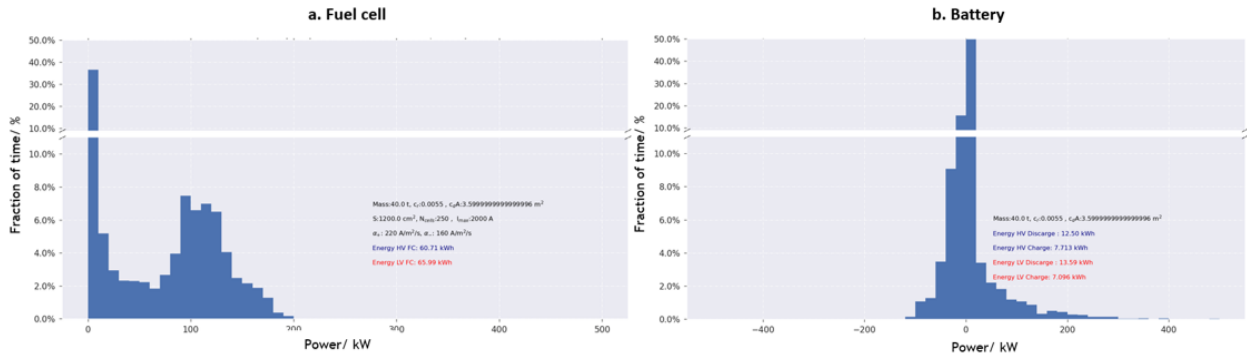


Figure 4.12. Histogram with the drive cycle time fraction spent in each power range for the FC and battery.

Power values of zero represent the moment when the vehicle is not demanding or producing energy, and both the FC and the LiB exhibit a high percentage of time spent in this stage (ca. 40 % and 50 % respectively). The FC exhibits also a significant fraction of time distributed in values of power between 100 kW and 200 kW.

Regarding the LiB, it has a higher portion of the time placed on negative values (from -100 kW to 0 kW). This occurs since the battery is advantageous, especially to avoid the FC damage when the power demand decreases.

Another important output from the simulator is the time fraction spent in each system efficiency value ($\varepsilon_{\text{system}}$) which was achieved using Equation (4.1), where $\dot{n}_{\text{H}_2, \text{st}}$ is the H₂ molar flow feed, and ΔH_{LHV} is the heat of the H₂ combustion and is assumed as 286 kJ mol⁻¹. The resultant plot for the example under consideration is presented in Figure 4.13.

$$\varepsilon_{\text{system}} = \frac{U_{\text{HV}} \cdot i_{\text{FC}, \text{HV}}}{\dot{n}_{\text{H}_2, \text{st}} \cdot \Delta H_{\text{LHV}}} \quad (4.1)$$

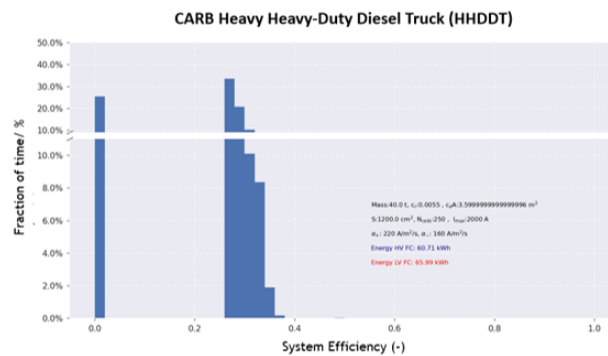


Figure 4.13. Histogram with the drive cycle time fraction spent in each system efficiency range for the FC.

It is possible to observe that the fraction of time spent in efficiencies close to zero is similar to the one on the FC power distribution (Figure 4.12.a). Also, the histogram shows that the most significant fraction of the time is spent in efficiency values of 0.3.

4.3 Hybrid strategy analysis

The final analysis using the simulator developed was the hybrid-strategy evaluation. Thus, three parameters were studied: α_+ , α_- , and the battery capacity.

Firstly, the simulator was run with different values of α_+ and α_- , assuming a default value of 93 600 A s for the battery capacity. This represents 6.5 times the battery capacity of a FC vehicle, such as a Toyota Mirai. The resultant $\varepsilon_{\text{system}}$, as well as the H_2 consumption were computed. The H_2 consumption was estimated through stoichiometry, while the $\varepsilon_{\text{system}}$ was achieved through Equation (4.1).

The results are presented as contour plots in Figure 4.14. Additionally, in each plot, two different zones can be distinguished. The pink ones represent zones where the power produced is lower than the power demand (there is some uncovered time), while in the green one, the total power demand is successfully produced by the FC / LiC hybrid system.

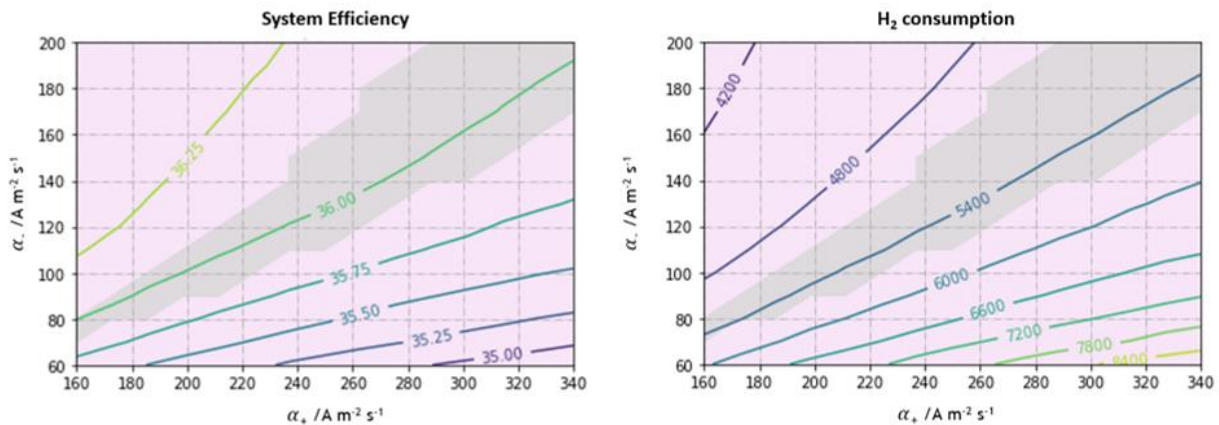


Figure 4.14. System efficiency and H_2 consumption contours assuming a battery capacity of 93 600 A s.

The contours show that the system efficiency can be improved by increasing the α_- or decreasing the α_+ . Thus, the H_2 consumption is higher for high values of α_+ and low α_- , where the system efficiency is lower. The two parameters may be adjusted to achieve high efficiencies and low H_2 consumption. However, the power demand must be accomplished, which means that the operating point must be inside of the green zone.

Another important factor to evaluate is the $T_{\text{min,rated}}$. As shown in Figure 4.15, the ideal operating temperature of 80 - 85 °C was achieved for α_- values of 100 - 170 $\text{A m}^{-2} \text{s}^{-1}$ and α_+ values of 220 - 260 $\text{A m}^{-2} \text{s}^{-1}$. It is also possible to observe that a higher α_- and lower α_+ results in lower operating $T_{\text{min,rated}}$, since the FC is allowed to decrease higher current values and increase lower current values.

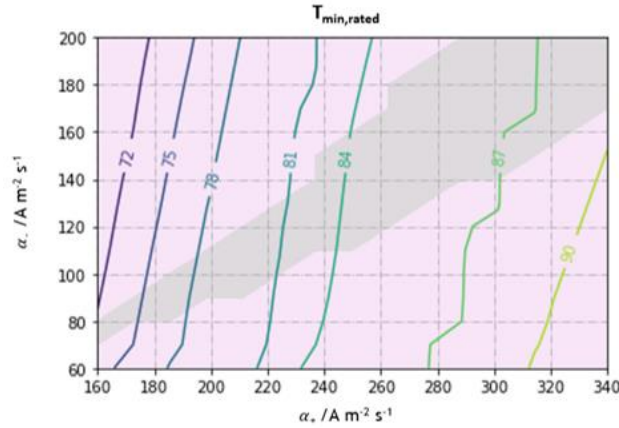


Figure 4.15. $T_{min,ated}$ contours for different values of α_+ and α_- assuming a battery capacity of 93 600 A s.

An ideal operating point must stay within the green zone and respect the temperature range of 80 - 85 °C. An example of three different operating conditions and the respective output analysis can be observed in Appendix J -. The study of the three examples confirmed the conclusions regarding the system efficiency, H_2 consumption, and $T_{min,ated}$. Additionally, it was possible to understand that by increasing α_- and decreasing α_+ the FC power demand decreases.

In fact, the FC and LiC energy demand were also analyzed for different values of α_- and α_+ , and the plots for the first parameter are graphically represented in Figure 4.16.

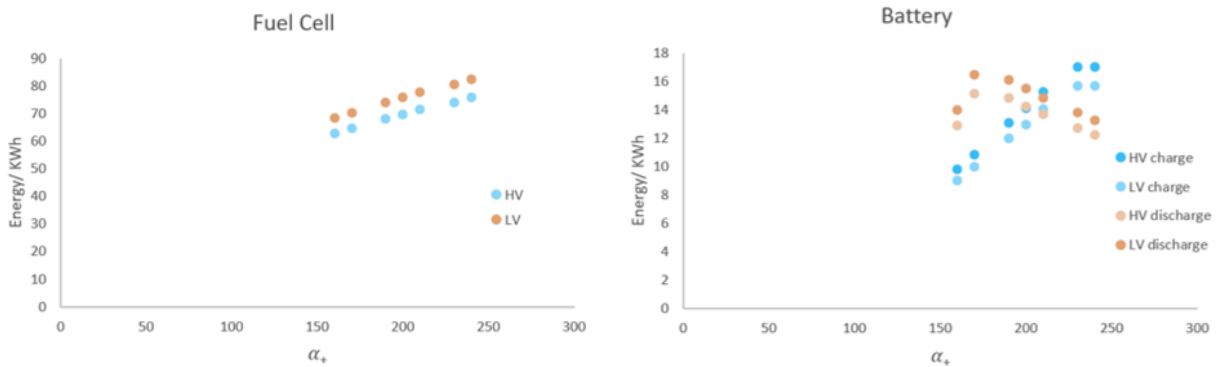


Figure 4.16. Energy demand from the FC and Battery for different values of α_+ .

The analysis of both graphs shows that increasing the α_+ value, the energy demand is higher for the FC and lower for the battery in discharging mode. On the other hand, in charging mode, the energy increases for higher values of α_+ . Hence, the increment of this parameter leads to an intensification of the dependency on the FC for the energy production.

The same plots were obtained for the α_- values and are displayed in Figure 4.17. Unlike the α_+ variation, the increment of the α_- value results in an energy demand lower for the FC and higher for the LiC. Still, in charging mode, the energy decreases for higher values of α_- . Thus, the power dependency on the battery is intensified by increasing the α_- values.

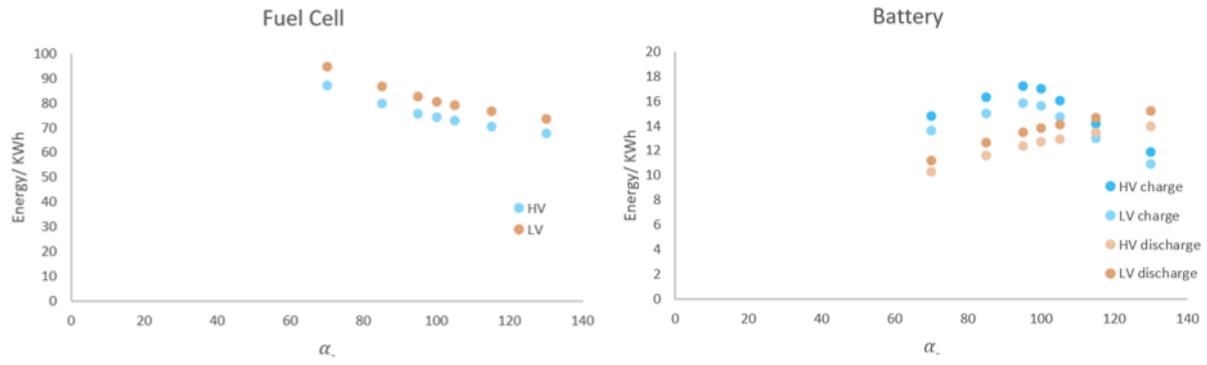


Figure 4.17. Energy demand from the FC and Battery for different values of α_- .

Regarding the battery capacity, a similar study was performed, and the results showed no significant influence on the resultant system efficiency, H_2 consumption, and $T_{\min, \text{rated}}$, as exhibited in Appendix K -. On the other hand, the battery capacity influences the uncovered time. A higher capacity results in a lower time uncovered. An example of this can be seen in Figure 4.18, where α_+ and α_- were considered as 230 and 140 $A m^{-2} s^{-1}$, respectively.

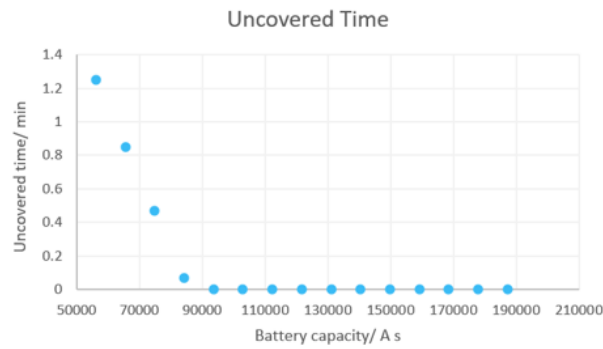


Figure 4.18. Time uncovered for different values of battery capacity, assuming constant α_+ and α_- as 230 and 140 $A m^{-2} s^{-1}$, respectively.

The battery capacity is defined by the needs of the FC. Thus, when the FC / LiB hybrid system is not able to produce the power demand, the battery can be switched by another one with a higher capacity, but it comprehends batteries more expensive.

Based on this information, it is possible to understand that it is important to find the optimal values of α_- and α_+ to take the best advantage of the FC. Still, the production of the required energy cannot be compromised, and the vehicle must complete the desired driving cycle. Therefore, the battery capacity can also be adjusted to achieve that.

These three parameters can be modified depending on the priorities, which can be the size of the FC or the battery, the total price, the H_2 consumption, among many others.

5 Conclusion

Within this project, new routines for a phenomenological model and simulator were developed. It is advantageous since it is focused on the FC / LiB vehicles, it is representative of the European heavy-duty class, and allows the user to specify many different properties regarding the vehicle, the FC stack, the battery and the expected drive cycle. Moreover, this is a convenient tool to compute the power demand, establish the hybrid strategy and estimate the H₂ consumption. This project was especially important for DLR since it will be further used on the stress tests definition for the FC.

On a first stage of the project, every kinetic parameter of the cycle, power demand values and the respective distribution along time were evaluated in order to find the most representative cycle of an EU heavy-duty vehicle. It was possible to confirm that the most suitable option was the RD cycle from VECTO library.

Using the selected cycle, it was possible to analyse the influence of the properties of the vehicle on the power demand. The results showed that N_E is more influenced by the powertrain efficiency and the mass load, while the R_E is more affected by the e and mass load. Both the e and mass load increment resulted in higher values of N_E and R_E . The powertrain efficiency increment did not influence the R_E and made the N_E decrease.

Also, the influence of each kinetic parameter on the effect of the properties of the vehicle on the power demand was studied. It was concluded that the v_{aero} was the kinetic parameter with the strongest influence. Increasing this parameter, the energy demand became more sensitive to variations in the properties of the vehicle.

With the simulator it was possible to estimate a decrease of 8.7 % and 12.0 % on R_E and N_E , respectively, in 5 to 8 years, considering the expected technological evolution established by the icct organization.

Regarding the power splitting strategy evaluation, the results showed that by decreasing the FC power production values (increasing α_- and decreasing α_+), the system efficiency increases and the $T_{min, rated}$ and H₂ consumption decreases. Also, it was observed that by increasing the battery capacity, the uncovered time decreases.

Consequently, the α_+ and α_- definition is an important step in the simulation to ensure the production of the power demand (avoiding uncovered time). If it is not possible, the battery can be switched by another one with higher capacity.

6 Assessment of the work done

6.1 Objectives achieved

The main objectives of this work were to help on the development of a new simulator and to use it to evaluate the drive cycle, the vehicle, the FC and the battery properties. The simulator was successfully upgraded.

Regarding the cycle analysis, it was possible to select the most representative one and the vehicle properties were properly analysed. The hybrid strategy was studied through the battery and the FC properties.

6.2 Other work carried out

Besides the core simulator, a user interface was also developed as secondary work. This was important to allow people without coding skills to use the simulator easily.

Due to time limitation, the FC analysis was not as complete as desired since its polarization curve was not evaluated. Therefore, it would be useful in the future to test different polarization curves in order to understand its effect on the power demand.

6.3 Final assessment

Working in a company like DLR was a great opportunity to work together with qualified people, from whom it was possible to learn a lot about PEMFC. Also, it became clear the potential of hydrogen as an energy source in the near future.

The four months at DLR-TT were important not only at a professional level, but also at a personal level. It was an important experience to earn responsibility and autonomy. Due to the time limitation, the project was an opportunity to work under pressures and high standards.

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Appendix A - Code example

The simulator developed on this project was structured in Spyder using Python. An example of the code can be observed in Figure A.1 and Figure A.2. This is a function that was developed to plot the FC system behaviour for different values of α_+ and α_- . An output example is shown in **Erro! A origem da referência não foi encontrada..**

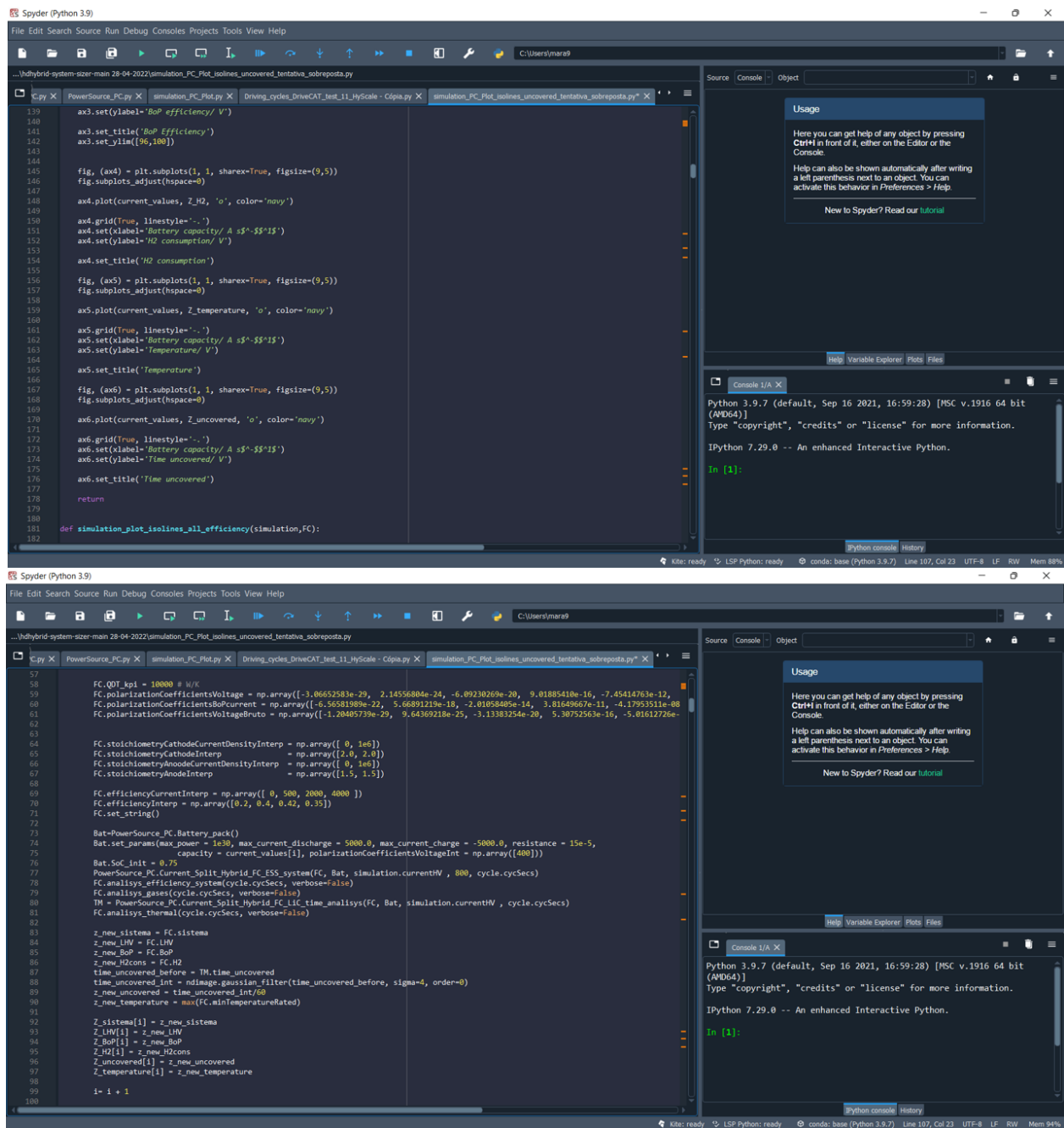


Figure A.1. Example of the code developed in the project, responsible for the plot of the FC behaviour for different α_+ and α_- values.

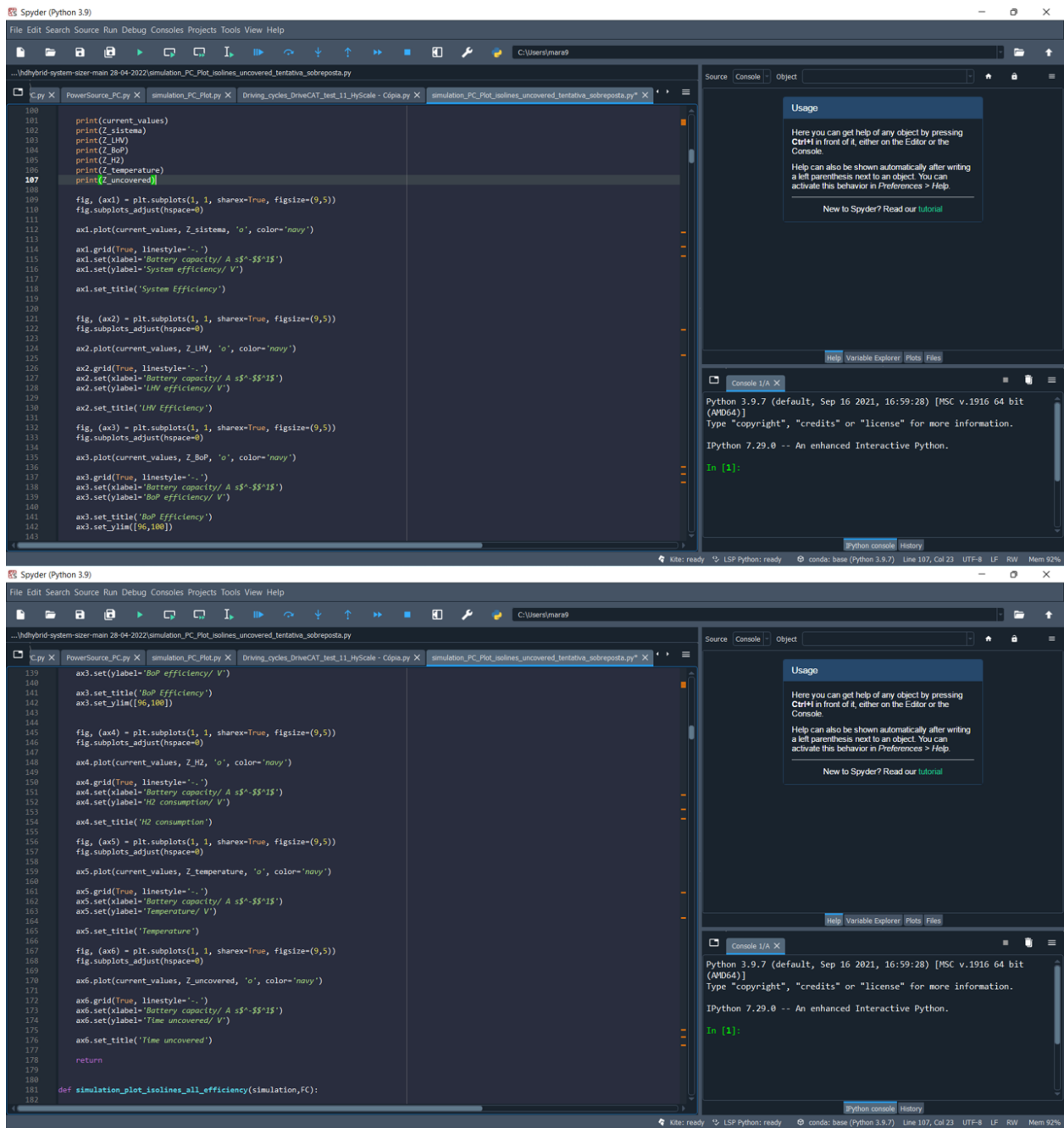


Figure A.2. Example of the code developed in the project, responsible for the plot of the FC behaviour for different α_+ and α_- values.

Appendix B - Default values for the vehicle's properties

In order to compare different driving cycles, some default values were considered for the vehicle properties. These were chosen accordingly to different past projects and research regarding heavy-duty vehicles emissions and considering the worst-case scenario where the maximum mass load is achieved. The values and respective references are exhibited in Table B.1.

Table B.1. Default values and respective references for vehicle properties.

Vehicle Property	Default Value	References
Vehicle mass empty/ kg	14 400	ICCT - 2017 ^[1]
Vehicle mass load/kg	25 600	ICCT - 2017 ^[1]
Vehicle rotational inertia factor/ (-)	1.05	ICCT - 2018 ^[2]
Vehicle frontal area/ m ²	6	ICCT - 2017 ^[1]
Vehicle drag coefficient/ (-)	0.6	ICCT - 2017 ^[1]
Vehicle rolling coefficient/ (-)	0.0055	ICCT - 2017 ^[1]
Vehicle powertrain efficiency/ (-)	0.9	Transportation Research - 2017 ^[3]
Vehicle converter efficiency/ (-)	0.9	MDPI - 2021 ^[4]

^[1] O. Delgado et al., "Fuel Efficiency Technology in European Heavy-Duty Vehicles: Baseline and Potential for the 2020-2030 Time Frame," 2017. [Online]. Available: www.theicct.org

^[2] F. Rodríguez, "Fuel Consumption Simulation of HDVS in the EU: Comparisons and Limitations," Mar. 2018. Available: www.theicct.org

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Appendix C - O₂ and H₂ moles stoichiometric

On the cathode layer of the FC, the Equation (2.3) occurs and the O₂ supplied reacts. The number of moles of O₂ consumed in a single FC ($\dot{n}_{FC,O_2}$) can be estimated through Equation (C.1), since the consumption of 1 mole of O₂ requires the consumption of 4 moles of e⁻ [31].

$$\dot{n}_{FC,O_2} = \frac{i_{FC,Bruto}}{4 \cdot F} \quad (C.1)$$

As there are several FC stacked together, the total O₂ moles consumed on the cathode ($\dot{n}_{O_2}$) is computed through Equation (C.2).

$$\dot{n}_{O_2} = NC \cdot \frac{i_{FC,Bruto}}{4 \cdot F} \quad (C.2)$$

On the anode layer of the FC, the Equation (2.2) occurs and the H₂ supplied reacts. The H₂ consumption in a single FC ($\dot{n}_{FC,H_2}$) can be estimated through Equation (C.3). The stoichiometric number translates that the consumption of 1 mol of H₂ results in the production of 2 moles of e⁻ [31].

$$\dot{n}_{FC,H_2} = \frac{i_{FC,Bruto}}{2 \cdot F} \quad (C.3)$$

The total H₂ moles consumed on the anode ($\dot{n}_{H_2}$) is estimated with Equation (C.4).

$$\dot{n}_{H_2} = NC \cdot \frac{i_{FC,Bruto}}{2 \cdot F} \quad (C.4)$$

Appendix D - Air compressor thermodynamics

Considering the air supplier operates in isentropic conditions, from the Carnot cycle the Equation (D.1) and (D.2) can be estimated. h represents the enthalpy and η the isentropic efficiency [71]-[73].

$$\eta = \frac{h_{2s} - h_1}{h_2 - h_1} \quad (D.1)$$

$$\frac{T_{2s}}{T_1} = \left(\frac{P_2}{P_1} \right)^{\frac{\gamma-1}{\gamma}} \quad (D.2)$$

From the Carnot cycle literature, it is possible to understand that the power required for the compressor can be computed through Equation (D.3) [71]-[73].

$$\dot{W} = (h_2 - h_1) \cdot \dot{m} \quad (D.3)$$

Considering ideal gases, Equation (D.4) can be estimated [71], [73].

$$\dot{W} = \frac{Cp_{air} \cdot T_1}{\mu} \cdot \left[\frac{T_{2s}}{T_1} - 1 \right] \cdot \dot{m} \quad (D.4)$$

Relating Equations (D.2) and (D.4) the power demand for the air compressor can be computed through Equation (D.5).

$$\dot{W} = \frac{Cp_{air} \cdot T_1}{\mu} \cdot \left[\left(\frac{P_2}{P_1} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right] \cdot \dot{m} \quad (D.5)$$

Appendix E - User interface

The user interface was developed in the Jupyter Notebook, the first stage of the program, the mechanical simulation is displayed in Figure E.1, Figure E.2, and Figure E.3. The second stage is presented in Figure E.4 and Figure E.5.

Software explanation:

This software is important to study the power demands and hybrid strategies.

In the first stage, it allows the user to choose the vehicle and drive-cycles to run the test. After that, it computes the power demand of the vehicle, exhibits the drive cycle, and computes the kinetics parameters associated.

The following stage starts with the user defining the efficiencies and specifications of the fuel cell and the battery/capacitor and the hybrid strategy.

Together with the information from the first stage, the software computes and specifies the energy required from the fuel cell and the battery/capacity.

User guide:

This document is a prototype of the user interface.

First, to initiate the software imports the modules needed.

Define the cycle:

To start the first stage described above, a drive cycle must be chosen.

The software allows the user to choose one drive cycle from a DriveCAT, FASTSim, or VECTO folder.

- **DriveCAT** cycle are defined by a number (0 to 32) in the variable "DriveCAT_cycle_number"

There is a list of 33 different driving cycles. This list was obtained from trucks, buses and light-duty vehicles.

As the goal of the simulation is to evaluate the power demand of a heavy-duty vehicle, some of the listed cycles are not considered since they are representative of light-duty cycles.

The software considers "unreasonable cycles" the ones exhibiting high-speed values (over 100 km/h) or intense acceleration resulting in extreme power values (over 400/450 kW).

Therefore, the available reasonable cycles are:

COACH-BUS

Empty mass below 33 000 lb (1 500 kg)

Number	COACH-BUS Drive Cycles Name
[1]	Arterial Segment of the Transit Coach Operating Duty Cycle
[2]	Braunschweig City Driving Cycle
[8]	Central Business District (CBD) Segment of the Transit Coach Operating Duty Cycle
[10]	Commuter Segment of the Transit Coach Operating Duty Cycle
[16]	Manhattan Bus Cycle 10Hz
[17]	New York Bus Composite Cycle (NY Comp)
[18]	New York Bus Cycle (NY Bus)
[31]	Orange County Transit Bus Cycle (US-OCTA) (California)

HEAVY-DUTY

Empty mass over 3 000 lb (1 500 kg)

Number	HEAVY-DUTY Drive Cycles Name
[4]	CARB Heavy Heavy-Duty Diesel Truck (HHDDT) Composite Cycle
[9]	City Suburban Heavy Vehicle Cycle (CSHVC)
[22]	NREL Neighborhood Refuse Truck Cycle
[23]	NREL Parcel Delivery Truck Cycle (Baltimore)
[24]	NREL Port Drayage Composite Cycle (California)
[29]	NREL Refuse Truck Cycle (Miami-Dade)
[30]	NREL Utility Truck Cycle (California)
[32]	Urban Dynamometer Driving Schedule for Heavy-Duty Vehicles (UDDS HD)
[33]	WVU 5-Peak Cycle

- **FASTSim** cycles are defined by their name "FastSIM_cycle_name".

There is a list of 4 options, which were collected from FastSIM programme sources.

Cycles available are:

Cycle Name
UDDS
US06
HWFET
longHaulDriveCycle_crop_4

Note:

Since different vehicles, with different specifications, achieve different targets, it is important to evaluate if the drive cycle is suitable for the vehicle under observation.

In other words, urban buses have higher acceleration values, compared with drayage trucks. However, they are also lighter and achieve lower speeds which allows them to accomplish the target speeds with reasonable power demands. A heavy drayage truck would need exaggerated power values to achieve the duty cycle of an urban bus.

With this in mind, it is important to choose one driving cycle out of the ones listed for the type of vehicle.

Define the Drive Cycle:

Figure E.1. User interface regarding the mechanical simulation.



Figure E.2. User interface regarding the vehicle simulation.

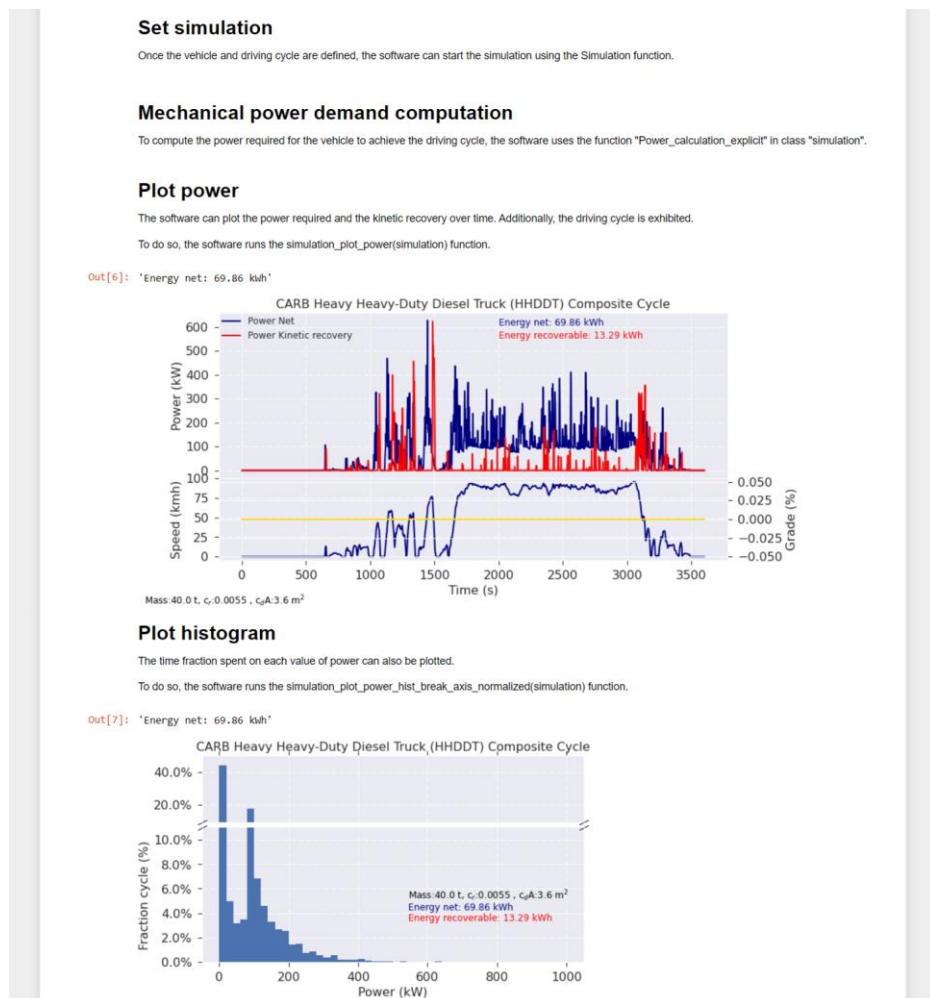


Figure E.3. User interface regarding the power demand computation.

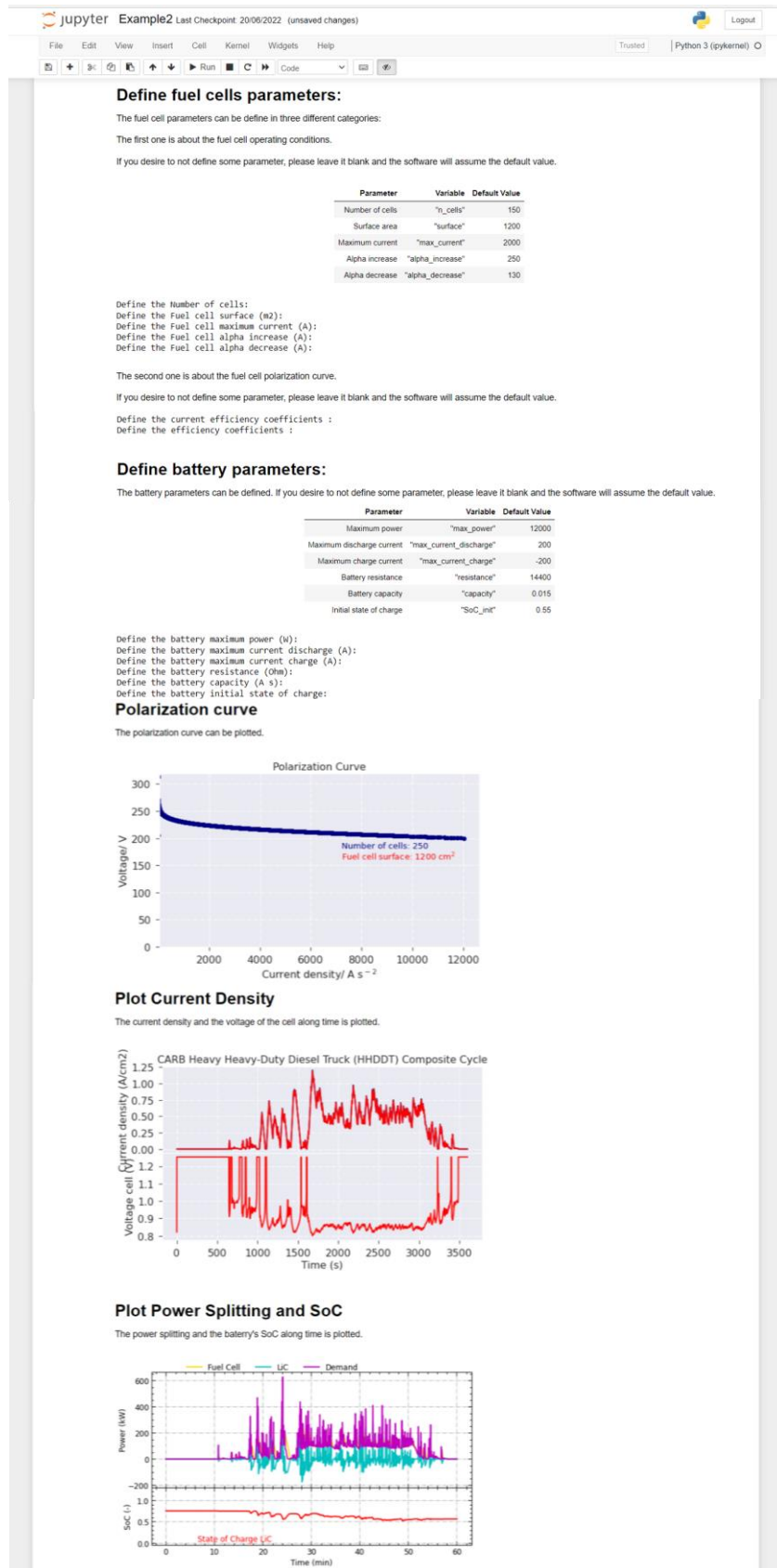


Figure E.4. User interface regarding the power splitting strategy.

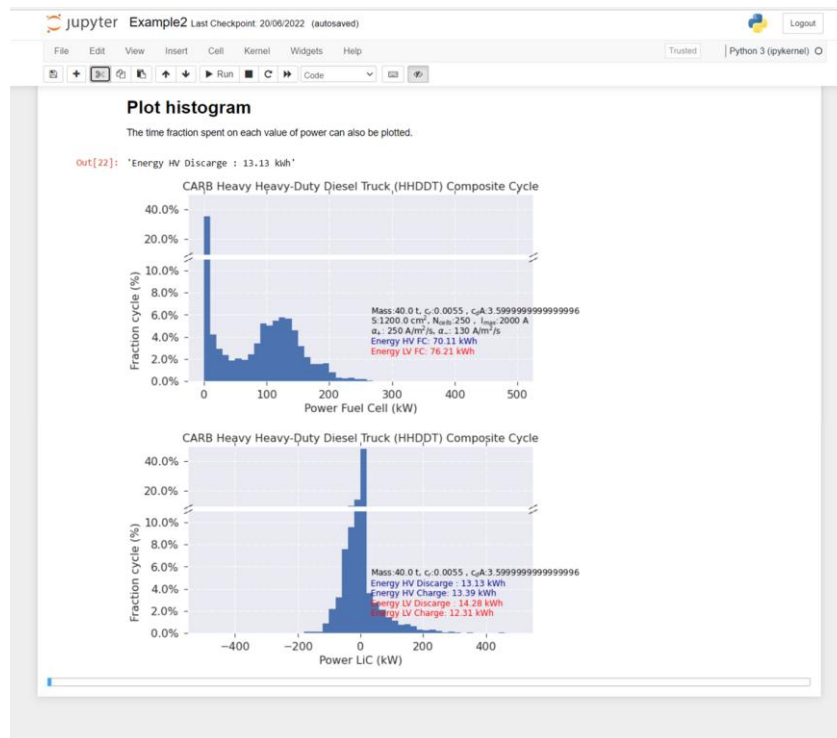


Figure E.5. User interface regarding the power splitting strategy.

Appendix F - Vehicle's properties effect

In order to analyze the effect of each vehicle property, a variation of Δd was made in every parameter and the power demand for each value was computed.

The NE and RE results for different values of vehicle mass empty considering the US cycle HHDDT are presented in Table F.1.

Table F.1. Values of NE and RE for different values of vehicle mass empty considering the US cycle (HHDDT).

Default Value/ kg	Δd / %	New Value/ kg	NE / kWh	RE / kWh
14 400	0	14 400	69.86	13.29
	+10	15 840	71.89	13.87
	-10	12 960	67.83	12.72
	+30	18 720	75.95	15.02
	-30	10 080	63.77	11.58

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +10 %, and +30 % is presented in Figure F.1.

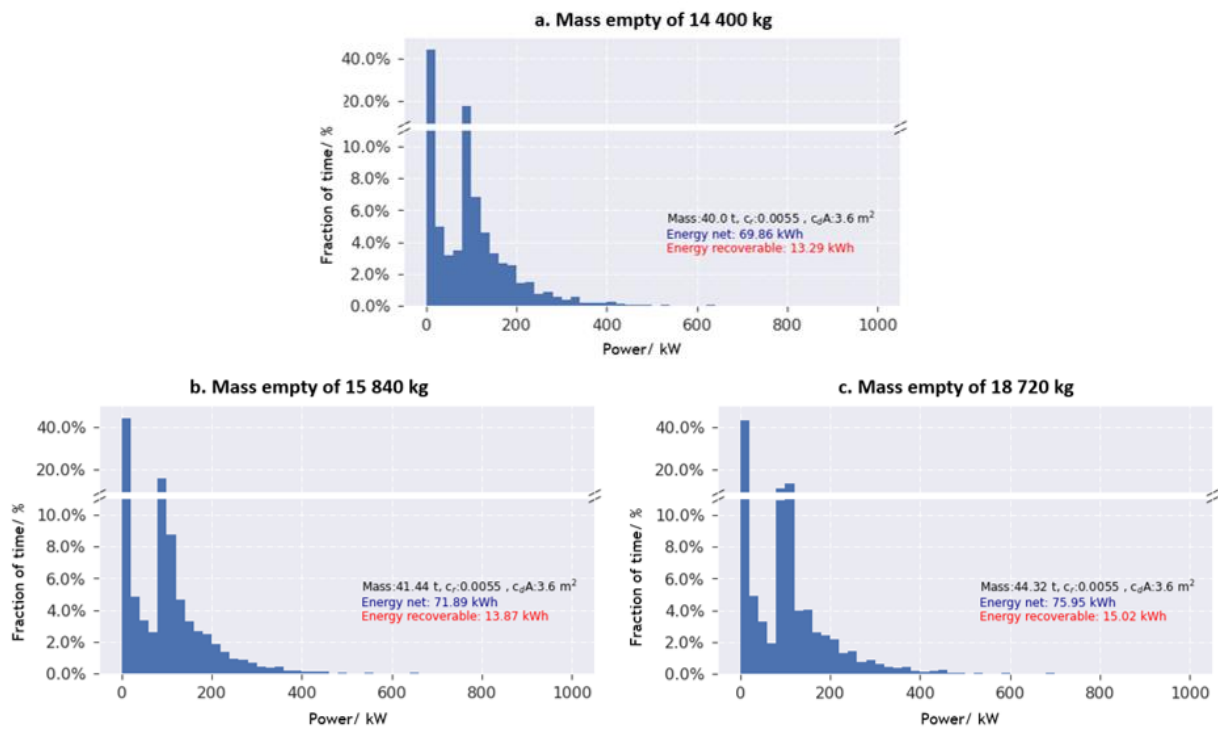


Figure F.1. Histogram with the drive cycle time spent in each power range for three different values of mass empty considering the US cycle (HHDDT).

In a similar way, the *NE* and *RE* results for different values of vehicle mass load are presented in Table F.2.

Table F.2. Values of *NE* and *RE* for different values of vehicle mass load considering the US cycle (HHDDT).

Default Value/ kg	Δd / %	New Value/ kg	<i>NE</i> / kWh	<i>RE</i> / kWh
25 600	0	25 600	69.86	13.29
	+10	28 160	73.38	14.25
	-10	23 040	66.34	12.34
	+30	33 280	80.43	16.19
	-30	17 920	59.30	10.44

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +10 %, and +30 % is presented in Figure F.2.

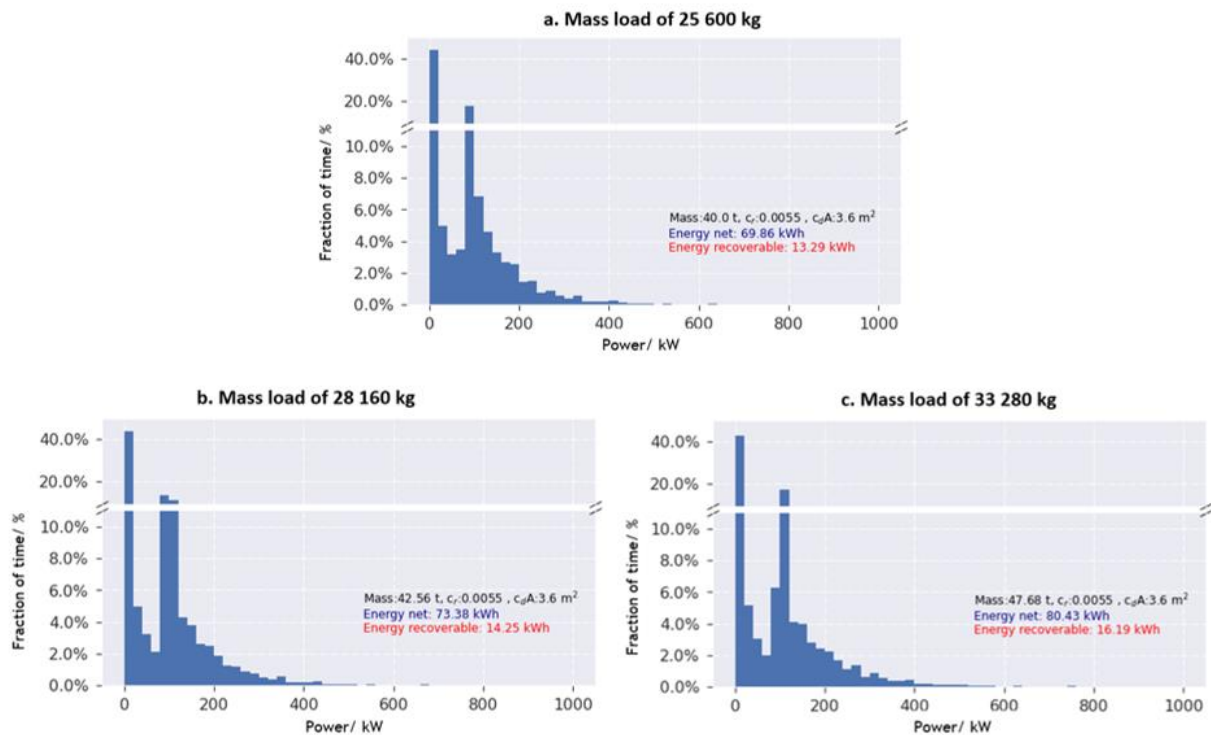


Figure F.2. Histogram with the drive cycle time spent in each power range for three different values of mass load considering the US cycle (HHDDT).

The vehicle rotational inertia factor variation was also analyzed by changing the Δd values presented in Table F.3.

Table F.3. Values of NE and RE for different values of vehicle inertial rotation factor considering the US cycle (HHDDT).

Default Value/ (-)	Δd / %	New Value/ (-)	NE/ kWh	RE/ kWh
1.050	0	1.050	69.86	13.29
	+5	1.103	70.38	13.67
	-5	0.998	69.35	12.93
	+10	1.155	70.89	14.04
	-10	0.945	68.84	12.56
	+30	1.365	72.94	15.56
	-30	0.735	66.79	11.14

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.3.

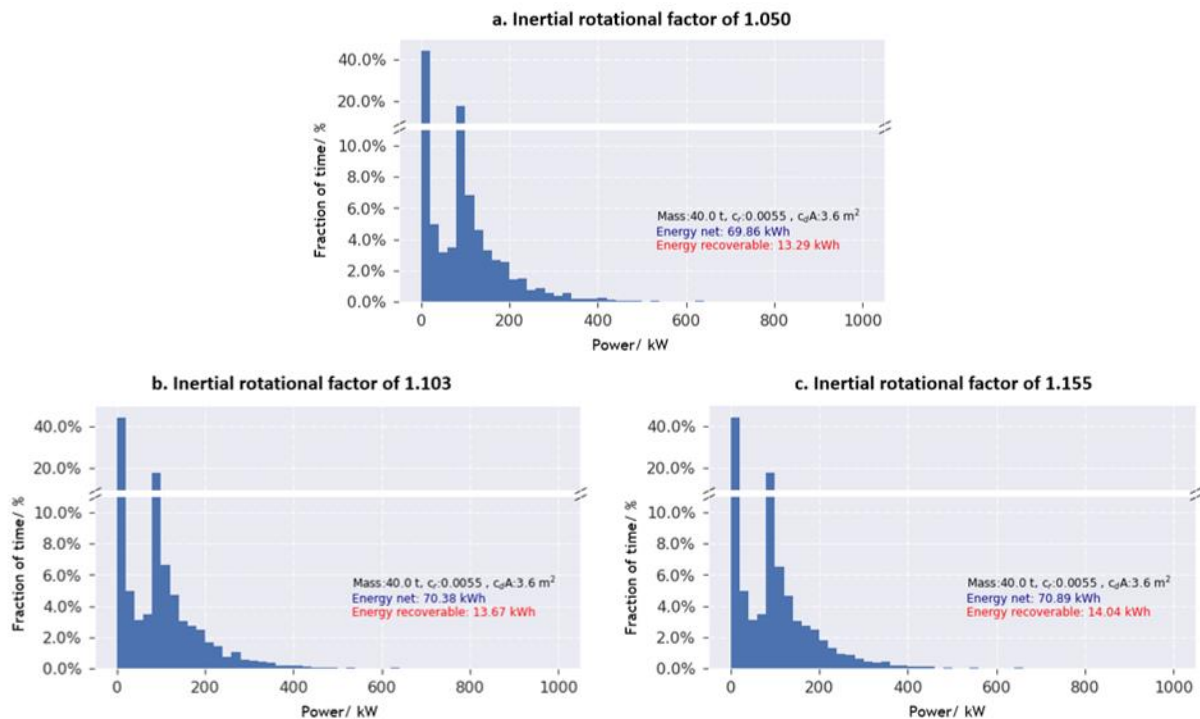


Figure F.3. Histogram with the drive cycle time spent in each power range for three different values of rotational inertia factor considering the US cycle (HHDDT).

Changing the vehicle frontal area by different values of Δd results in a variation of NP and RP as presented in Table F.4.

Table F.4. Values of NE and RE for different values of vehicle frontal area considering the US cycle (HHDDT).

Default Value/ m ²	Δd / %	New Value/ m ²	NE / kWh	RE / kWh
6.0	0	6.0	69.86	13.29
	+5	6.3	70.58	13.19
	-5	5.7	69.14	13.39
	+10	6.6	71.30	13.09
	-10	5.4	68.433	13.50
	+30	7.8	74.17	12.74
	-30	4.2	65.55	13.95

<The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.4.

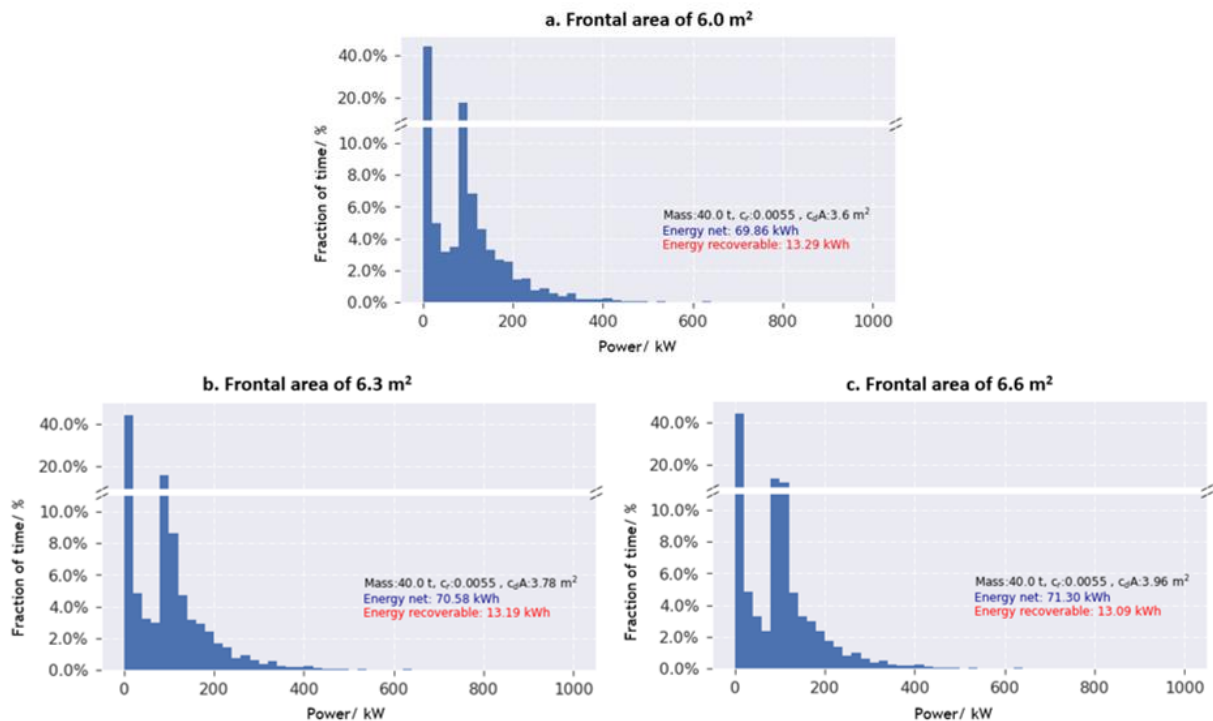


Figure F.4. Histogram with the drive cycle time spent in each power range for three different values of frontal area considering the US cycle (HHDDT).

The vehicle drag coefficient variation was also analyzed by changing the Δd values presented in Table F.5.

Table F.5. Values of NE and RE for different values of vehicle drag coefficient considering the US cycle (HHDDT).

Default Value/ (-)	Δd / %	New Value/ (-)	NE/ kWh	RE/ kWh
0.60	0	0.60	69.86	13.29
	+5	0.63	70.58	13.19
	-5	0.57	69.14	13.39
	+10	0.66	71.30	13.09
	-10	0.54	68.43	13.50
	+30	0.78	74.17	12.74
	-30	0.42	65.55	13.95

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.5.

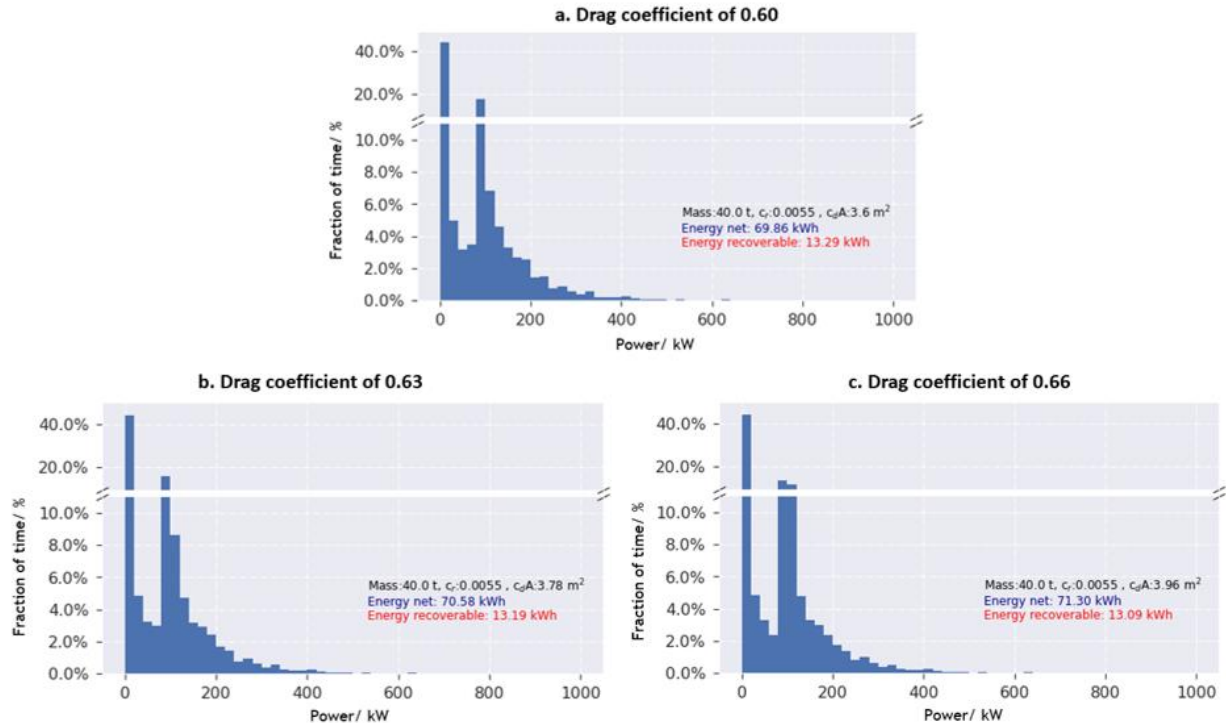


Figure F.5. Histogram with the drive cycle time spent in each power range for three different values of drag coefficient considering the US cycle (HHDDT).

The vehicle rolling coefficient variation was also analyzed by changing the Δd values presented in Table F.6.

Table F.6. Values of NE and RE for different values of vehicle rolling coefficient considering the US cycle (HHDDT).

Default Value/ (-)	Δd / %	New Value/ (-)	NE/ kWh	RE/ kWh
0.00550	0	0.00550	69.86	13.29
	+5	0.00578	71.74	12.99
	-5	0.00523	68.49	13.52
	+10	0.00605	72.65	12.85
	-10	0.00495	67.65	13.77
	+30	0.00715	78.23	12.06
	-30	0.00385	61.49	14.82

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.6.

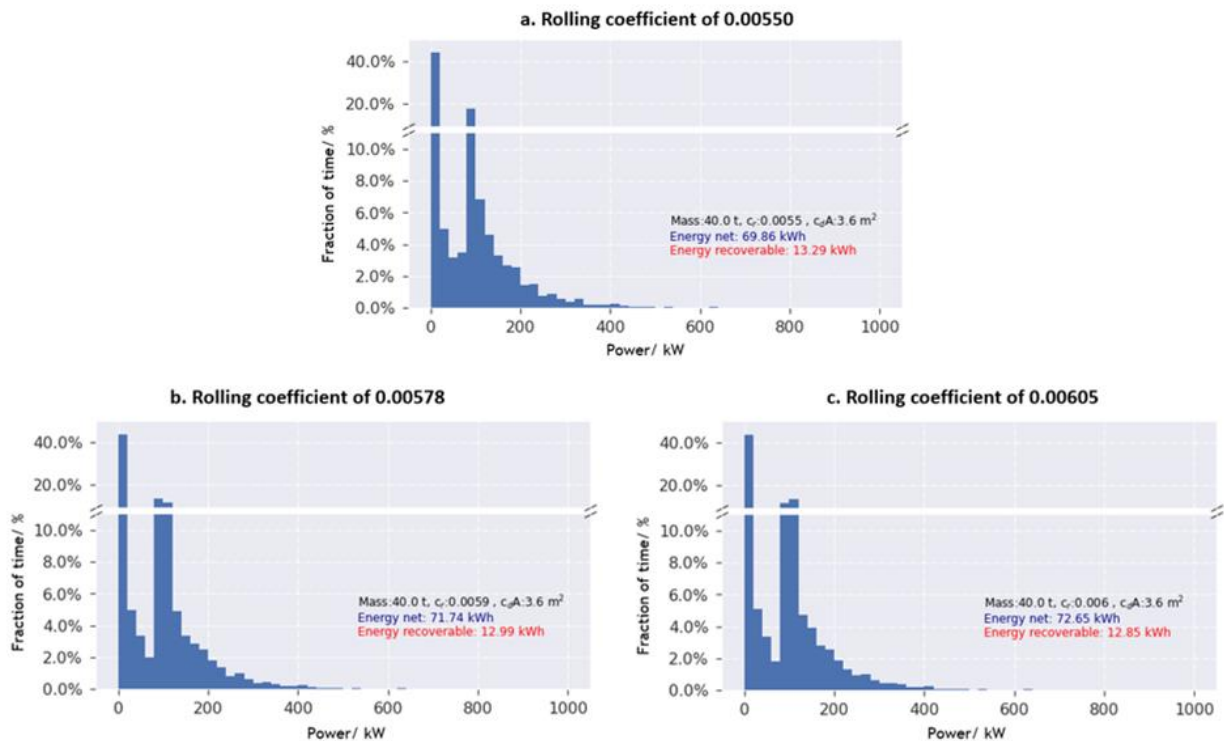


Figure F.6. Histogram with the drive cycle time spent in each power range for three different values of rolling coefficient considering the US cycle (HHDDT).

The vehicle powertrain efficiency coefficient variation was also analyzed by changing the Δd values presented in Table F.7.

Table F.7. Values of NE and RE for different values of vehicle powertrain efficiency considering the US cycle (HHDDT).

Default Value/ (-)	Δd / %	New Value/ (-)	NE/ kWh	RE/ kWh
0.90	0	0.90	69.86	13.29
	+5	0.95	66.53	13.29
	-5	0.86	73.54	13.29
	+7	0.96	65.29	13.29
	-7	0.84	75.12	13.29
	+10	0.99	63.51	13.29
	-10	0.81	77.62	13.29

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.7.

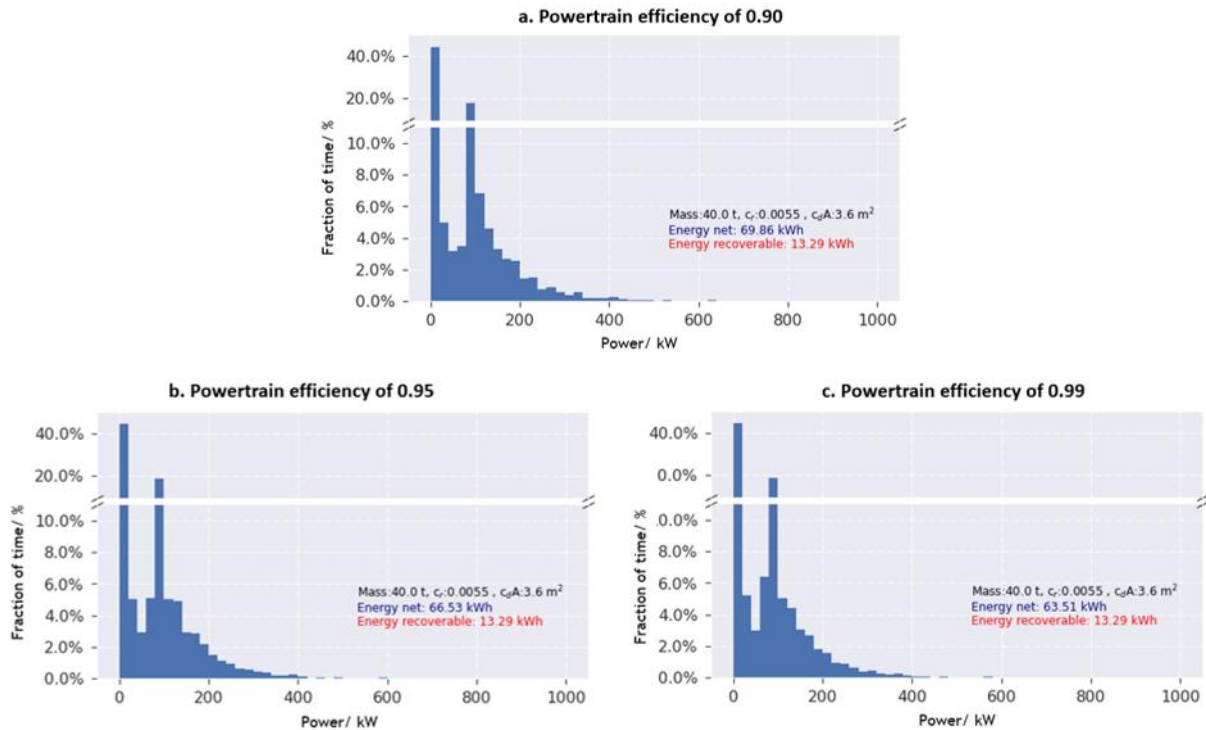


Figure F.7. Histogram with the drive cycle time spent in each power range for three different values of powertrain efficiency considering the US cycle (HHDDT).

The vehicle converter efficiency coefficient variation was also analyzed by changing the Δd values presented in Table F.8. Here it is possible to see that the converter efficiency does not influence the power demand.

Table F.8. Values of NE and RE for different values of vehicle converter efficiency considering the US cycle (HHDDT).

Default Value/ (-)	$\Delta d/ \%$	New Value/ (-)	NE/ kWh	RE/ kWh
0.90	0	0.90	69.86	13.29
	+5	0.95	69.86	13.29
	-5	0.86	69.86	13.29
	+7	0.96	69.86	13.29
	-7	0.84	69.86	13.29
	+10	0.99	69.86	13.29
	-10	0.81	69.86	13.29

The evolution of the net energy (NE) and recoverable energy (RE) variation over the property variation for the HHDDT cycle is presented in Figure F.8.

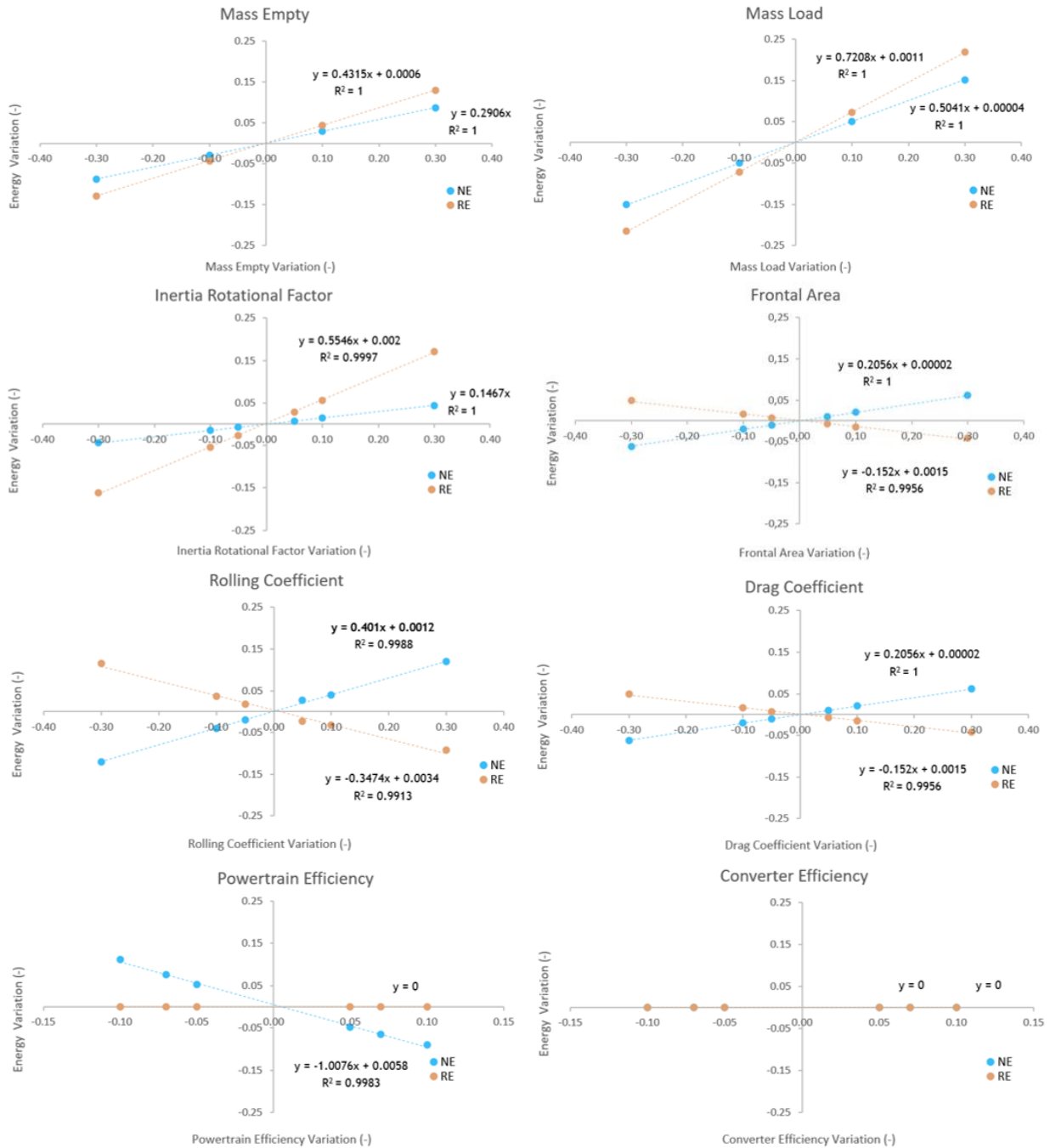


Figure F.8. The NE and RE variation along each vehicle property variation aiming the analysis of the vehicle properties' effect on power demand considering the US cycle (HHDDT).

A similar evaluation was done considering the EU cycle (RD). The NE and RE results for different values of vehicle mass empty are presented in Table F.9.

Table F.9. Values of *NE* and *RE* for different values of vehicle mass empty considering the EU cycle (RD).

Default Value/ kg	Δd / %	New Value/ kg	<i>NE</i> / kWh	<i>RE</i> / kWh
14 400	0	14 400	178.10	55.80
	+10	15 840	183.80	58.13
	-10	12 960	172.50	53.47
	+30	18 720	195.00	62.78
	-30	10 080	161.20	48.82

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +10 %, and +30 % is presented in Figure F.9.

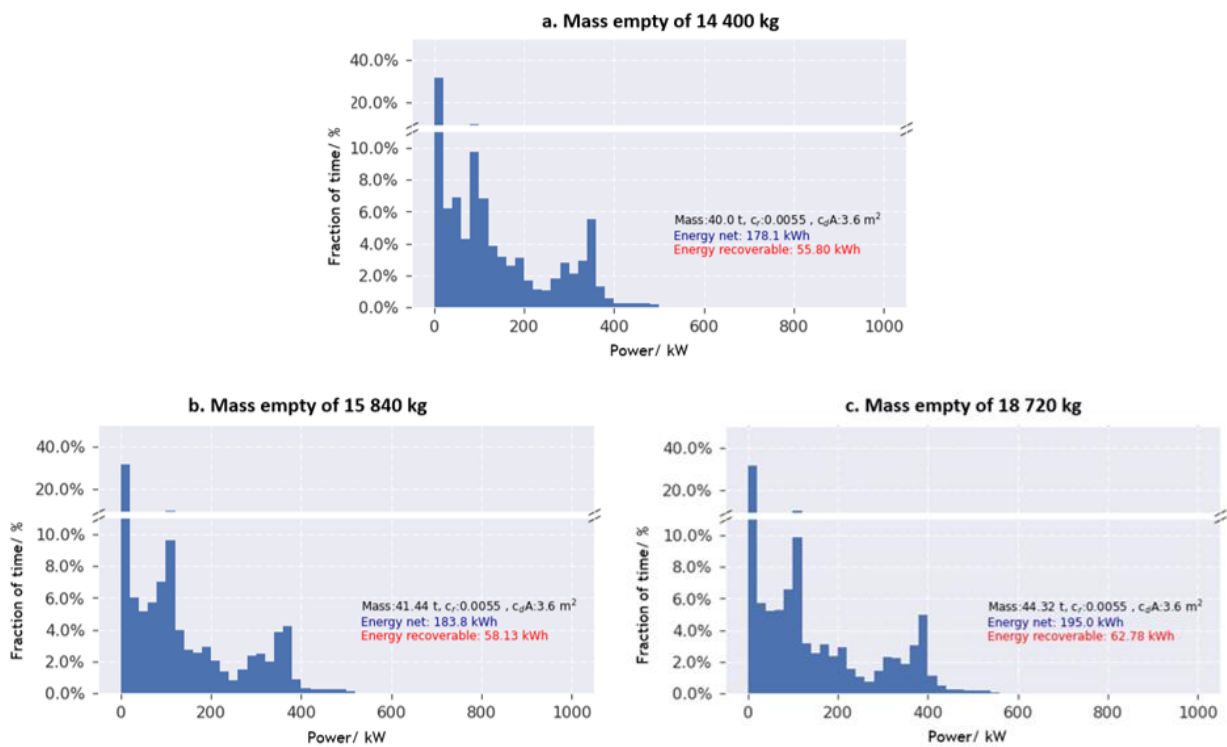


Figure F.9. Histogram with the drive cycle time spent in each power range for three different values of mass empty considering the EU cycle (RD).

In a similar way, the *NE* and *RE* results for different values of vehicle mass load are presented in Table F.10.

Table F.10. Values of NE and RE for different values of vehicle mass load considering the EU cycle (RD).

Default Value/ kg	Δd / %	New Value/ kg	NE / kWh	RE / kWh
25 600	0	25 600	178.10	55.80
	+10	28 160	188.00	59.84
	-10	23 040	168.20	51.75
	+30	33 280	207.80	67.93
	-30	17 920	148.50	43.69

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +10 %, and +30 % is presented in Figure F.10.

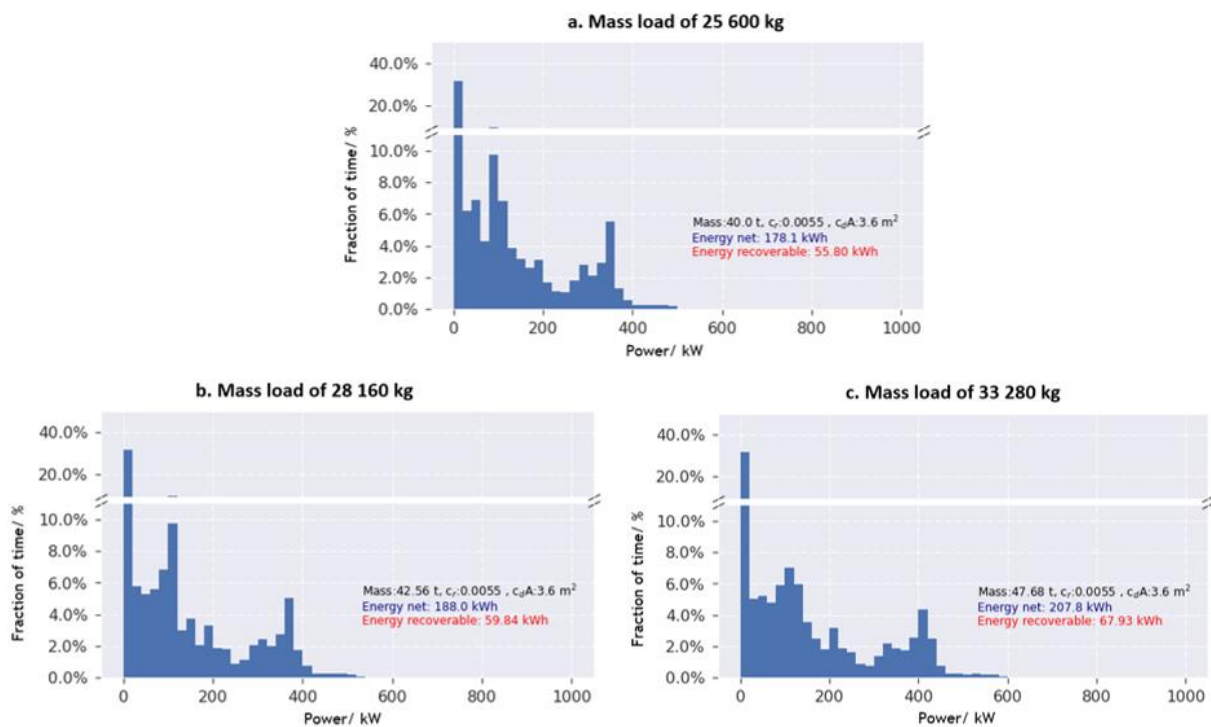


Figure F.10. Histogram with the drive cycle time spent in each power range for three different values of mass load considering the EU cycle (RD).

The vehicle rotational inertia factor variation was also analyzed by changing the Δd values presented in Table F.11.

Table F.11. Values of NE and RE for different values of vehicle inertial rotation factor considering the EU cycle (RD).

Default Value/ (-)	$\Delta d/ \%$	New Value/ (-)	NE/ kWh	RE/ kWh
1.050	0	1.050	178.10	55.80
	+5	1.103	178.90	56.37
	-5	0.998	177.30	55.24
	+10	1.155	179.70	56.93
	-10	0.945	176.50	54.67
	+30	1.365	182.90	59.21
	-30	0.735	173.30	52.44

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.11.

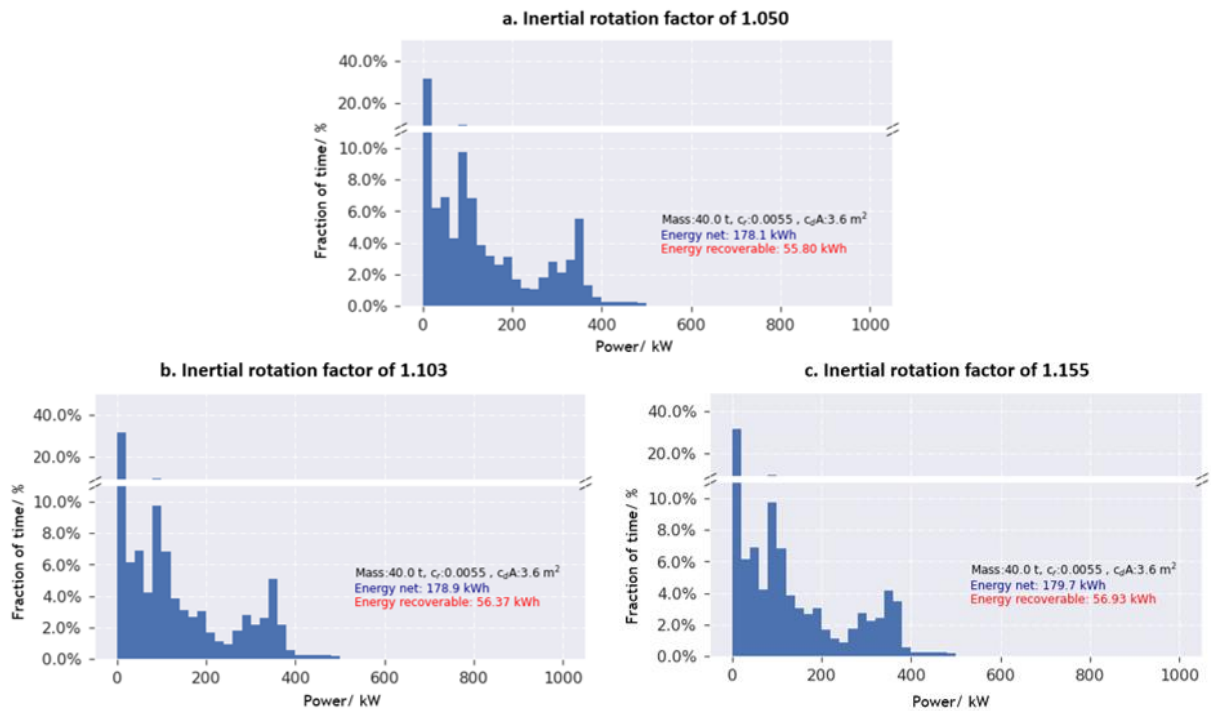


Figure F.11. Histogram with the drive cycle time spent in each power range for three different values of inertial rotation factor considering the EU cycle (RD).

Changing the vehicle frontal area by different values of Δd results in a variation of NP and RP as presented in Table F.12.

Table F.12. Values of NE and RE for different values of vehicle frontal area considering the EU cycle (RD).

Default Value/ (-)	Δd / %	New Value/ m ²	NE/ kWh	RE/ kWh
6.0	0	6.0	178.10	55.80
	+5	6.3	179.30	55.40
	-5	5.7	177.00	56.19
	+10	6.6	180.40	55.01
	-10	5.4	175.80	56.59
	+30	7.8	185.10	53.46
	-30	4.2	171.30	58.19

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.12.

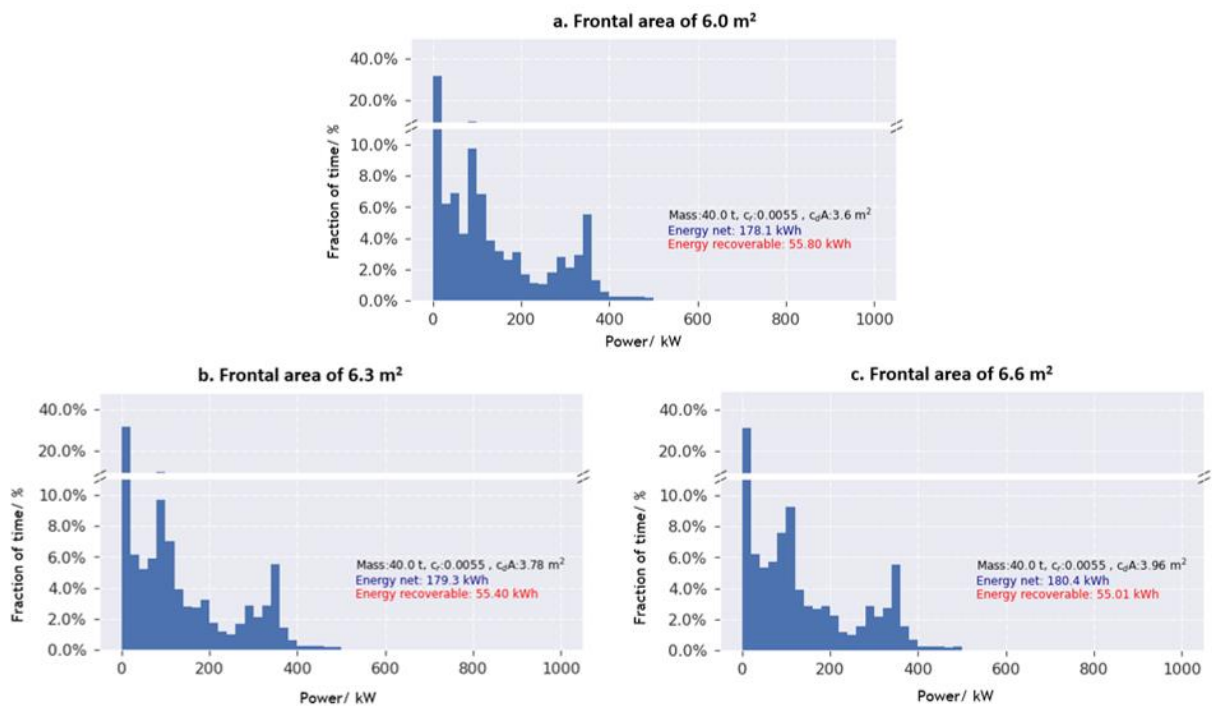


Figure F.12. Histogram with the drive cycle time spent in each power range for three different values of the frontal area considering the EU cycle (RD).

The vehicle drag coefficient variation was also analyzed by changing the Δd values presented in Table F.13.

Table F.13. Values of NE and RE for different values of vehicle drag coefficient considering the EU cycle (RD).

Default Value/ (-)	Δd / %	New Value/ (-)	NE/ kWh	RE/ kWh
0.60	0	0.60	178.10	55.80
	+5	0.63	179.30	55.40
	-5	0.57	177.00	56.19
	+10	0.66	180.40	55.01
	-10	0.54	175.80	56.59
	+30	0.78	185.10	53.46
	-30	0.42	171.30	58.19

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.13.

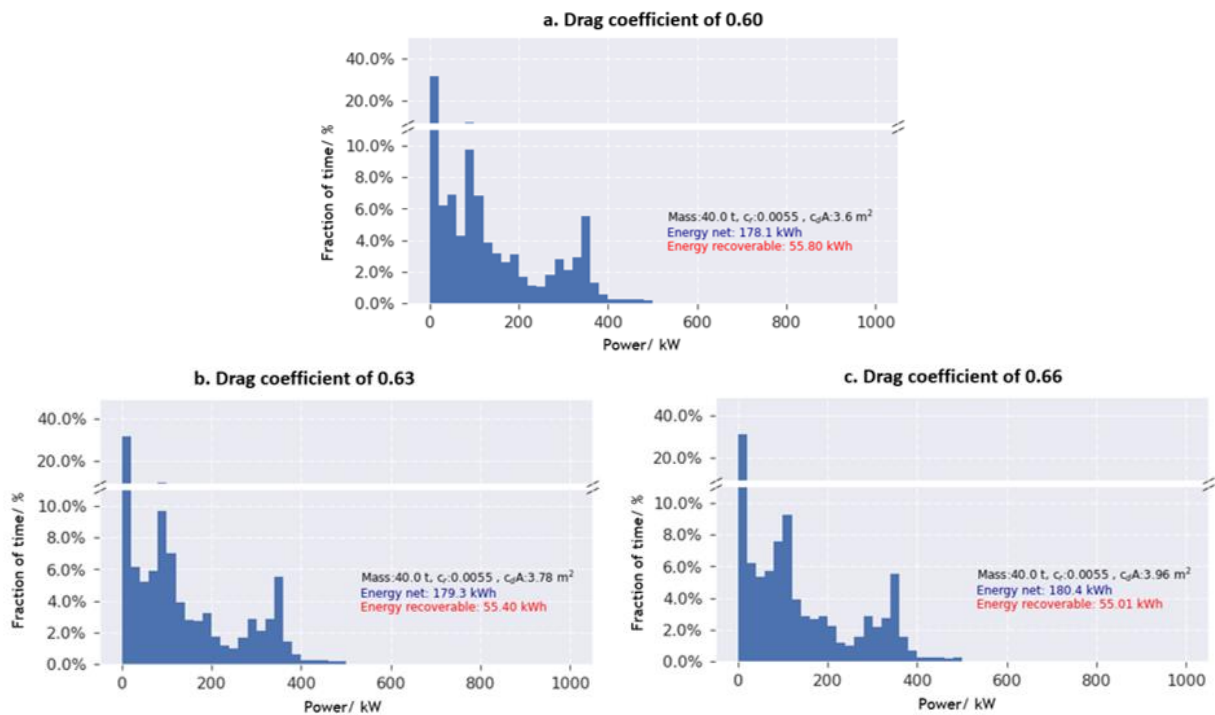


Figure F.13. Histogram with the drive cycle time spent in each power range for three different values of drag coefficient considering the EU cycle (RD).

The vehicle rolling coefficient variation was also analyzed by changing the Δd values presented in Table F.14.

Table F.14. Values of NE and RE for different values of vehicle rolling coefficient considering the EU cycle (RD).

Default Value/ (-)	Δd / %	New Value/ (-)	NE/ kWh	RE/ kWh
0.00550	0	0.00550	178.10	55.80
	+5	0.00578	180.80	54.89
	-5	0.00523	175.60	56.67
	+10	0.00605	183.40	54.03
	-10	0.00495	172.90	57.59
	+30	0.00715	194.00	50.58
	-30	0.00385	162.80	61.38

The vehicle powertrain efficiency coefficient variation was also analyzed by changing the Δd values presented in Figure F.14.

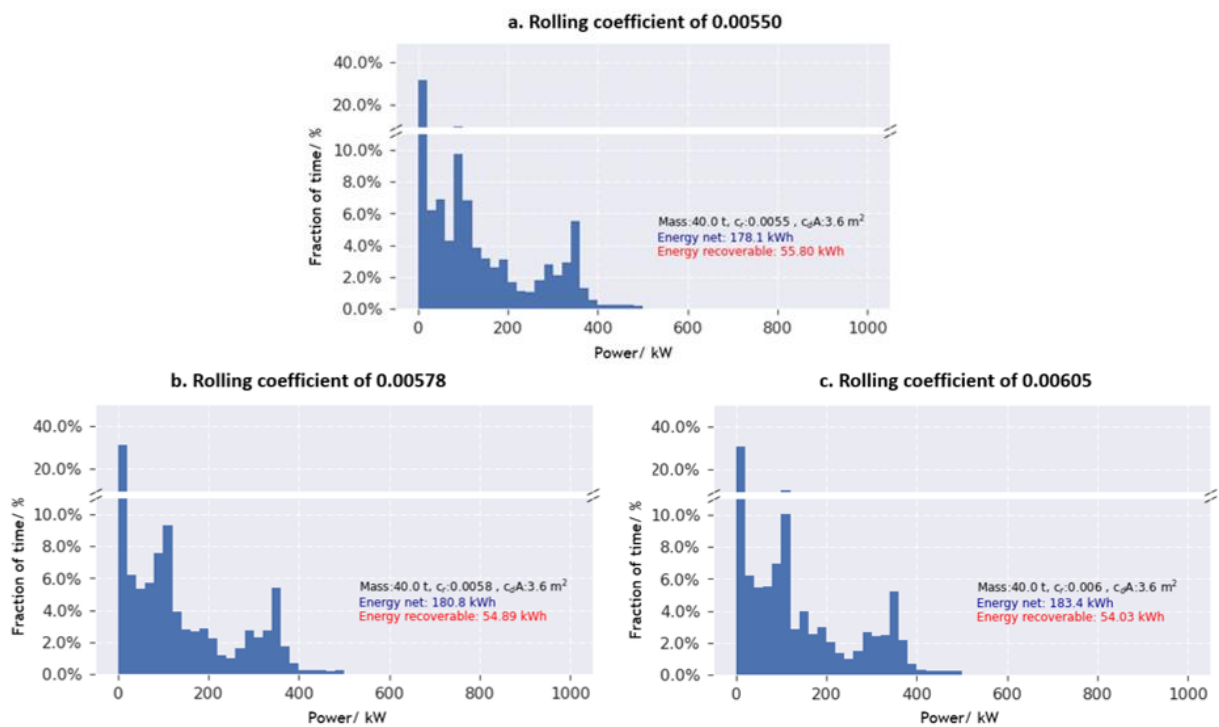


Figure F.14. Histogram with the drive cycle time spent in each power range for three different values of rolling coefficient considering the EU cycle (RD).

The vehicle powertrain efficiency coefficient variation was also analyzed by changing the Δd values presented in Table F.15.

Table F.15. Values of NE and RE for different values of vehicle powertrain efficiency considering the EU cycle (RD).

Default Value/ (-)	Δd / %	New Value/ (-)	NE/ kWh	RE/ kWh
0.90	0	0.90	178.10	55.80
	+5	0.95	169.60	55.80
	-5	0.86	187.50	55.80
	+10	0.96	166.50	55.80
	-10	0.84	191.50	55.80
	+30	0.99	161.50	55.80
	-30	0.81	197.70	55.80

The resulting histogram of the fraction of time spent in each power range for a Δd value of 0 %, +5 %, and +10 % is presented in Figure F.15.

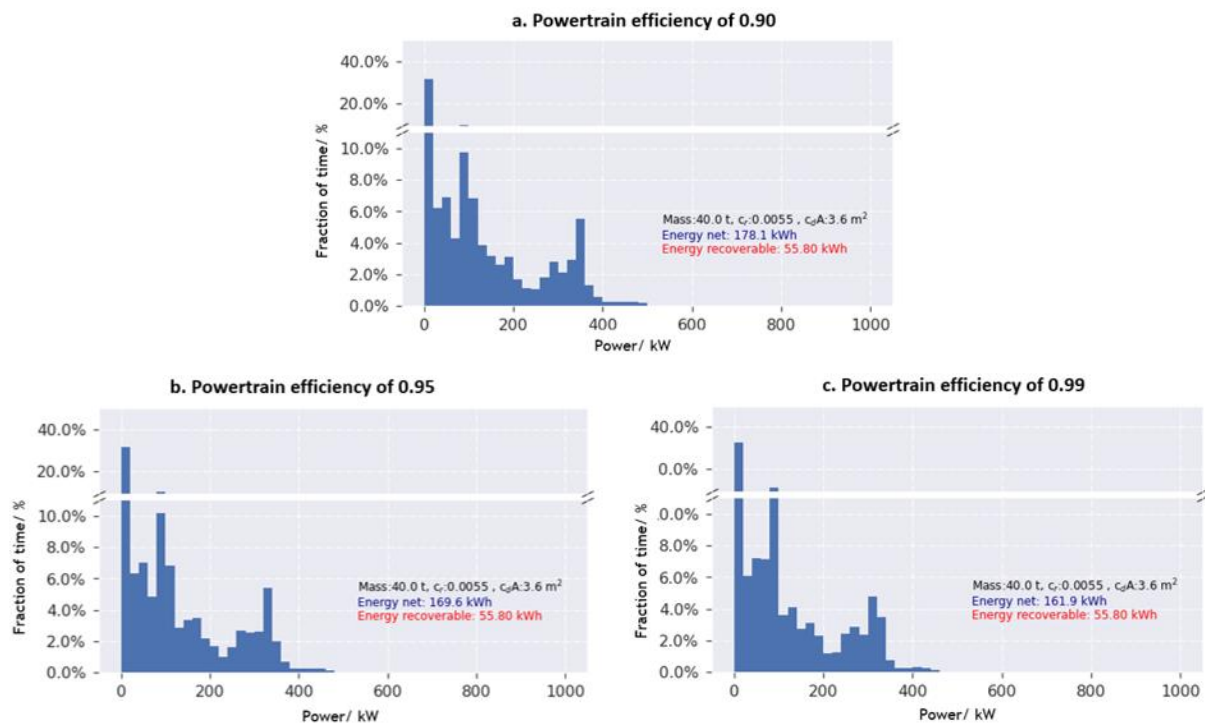


Figure F.15. Histogram with the drive cycle time spent in each power range for three different values of powertrain efficiency considering the EU cycle (RD).

The vehicle converter efficiency coefficient variation was also analyzed by changing the Δd values presented in Table F.16. Here it is possible to see that the converter efficiency does not influence the power demand.

Table F.16. Values of NE and RE for different values of vehicle converter efficiency considering the EU cycle (RD).

Default Value/ (-)	$\Delta d/ \%$	New Value/ (-)	NE/ kWh	RE/ kWh
0.90	0	0.90	178.10	55.80
	+5	0.95	178.10	55.80
	-5	0.86	178.10	55.80
	+10	0.96	178.10	55.80
	-10	0.84	178.10	55.80
	+30	0.99	178.10	55.80
	-30	0.81	178.10	55.80

Appendix G - Cycle's properties influence

In order to understand the cycle parameters' influence in the relation between the energy demand, each kinetic parameter and six cycles were evaluated: HHDDT, California, UDDS HV, LHDC, LH, and RD. The results can be observed in the following figures.

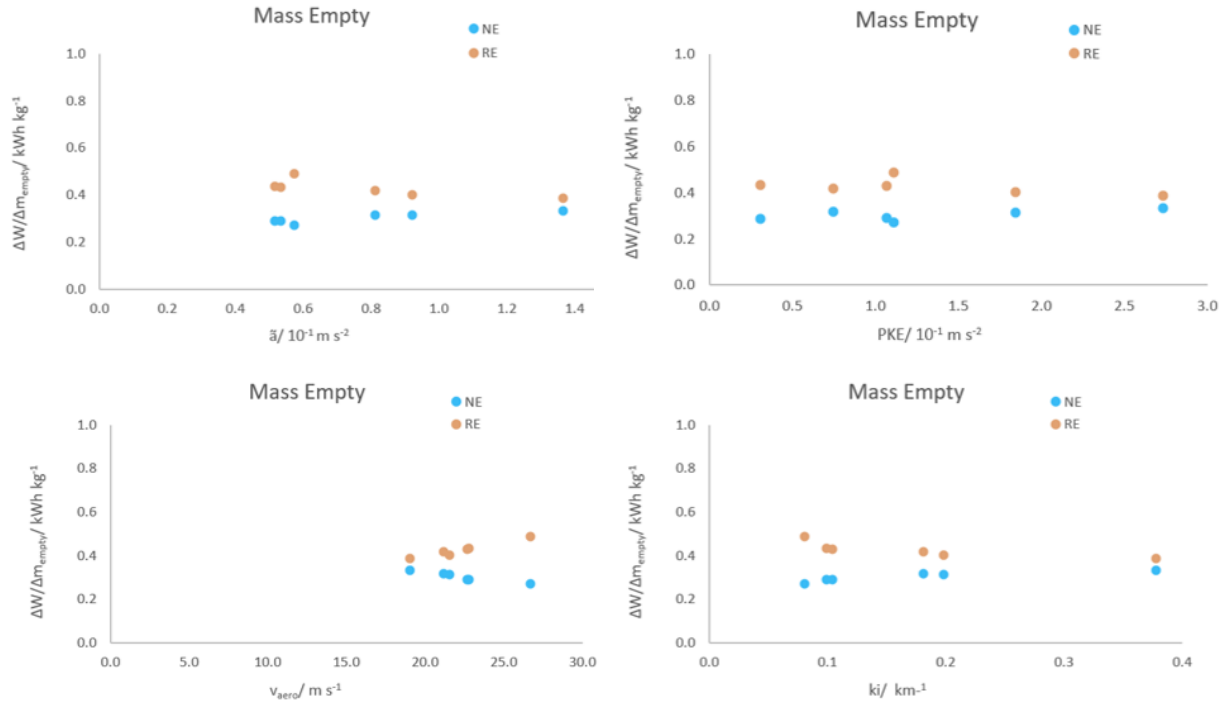


Figure G.1. Graphical representation of the relation between the energy variation and the mass empty ($\Delta W / \Delta m_{empty}$) for different values of the cycle parameters: PKE , $\tilde{a}$, v_{aero} , and ki .

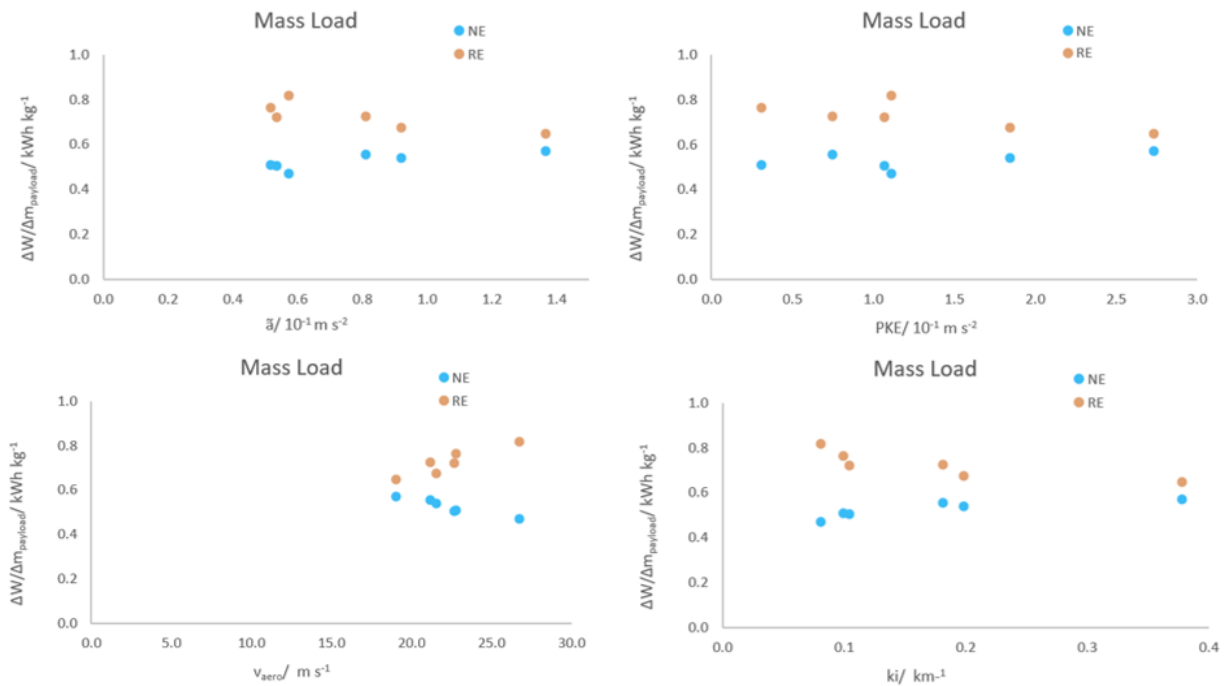


Figure G.2. Graphical representation of the relation between the energy variation and the mass load ($\Delta W / \Delta m_{payload}$) for different values of the cycle parameters: $\tilde{a}$, PKE , v_{aero} , and ki .

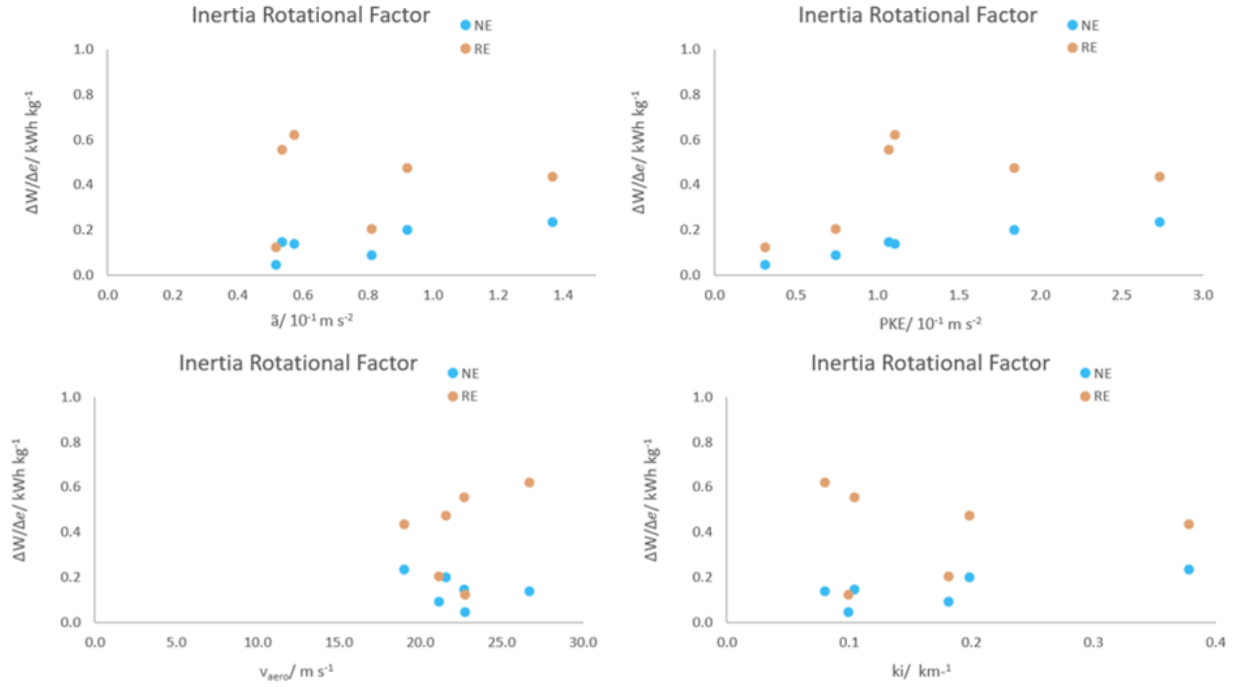


Figure G.3. Graphical representation of the relation between the energy variation and the vehicle inertial rotation factor ($\Delta W / \Delta e$) for different values of the cycle parameters: PKE , $\tilde{a}$, v_{aero} , and ki .

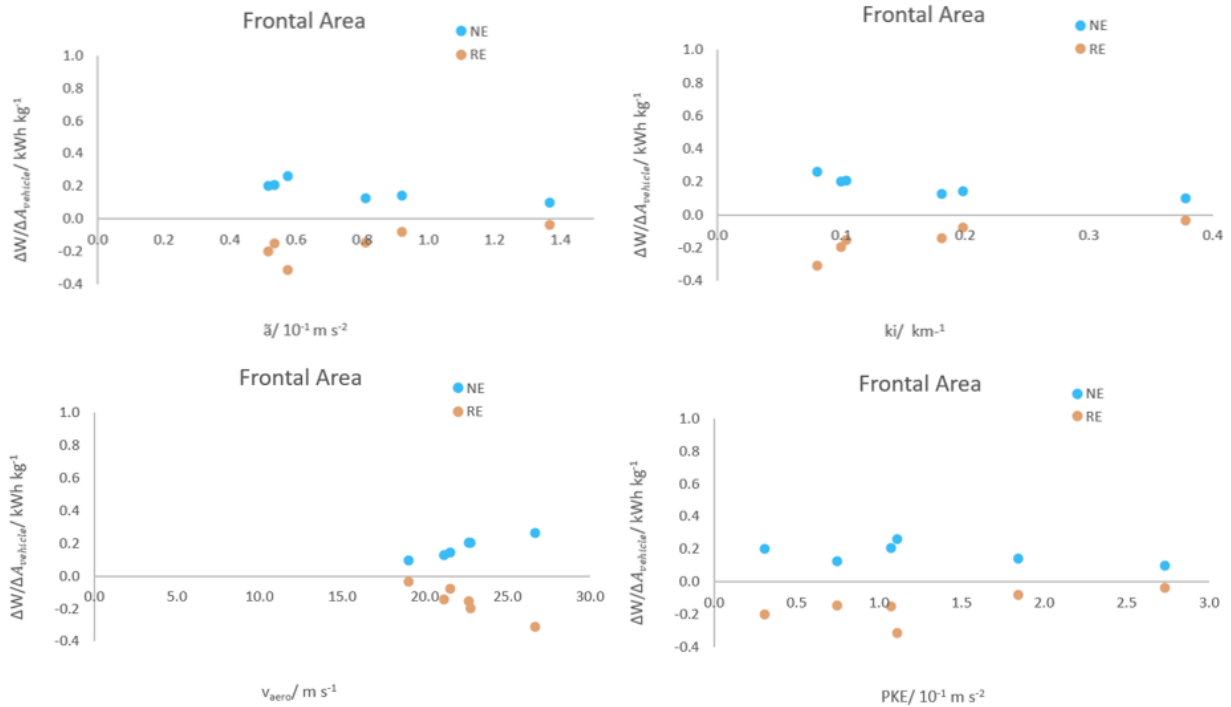


Figure G.4. Graphical representation of the relation between the energy variation and the vehicle frontal area ($\Delta W / \Delta A_{vehicle}$) for different values of the cycle parameters: PKE , $\tilde{a}$, v_{aero} , and ki .

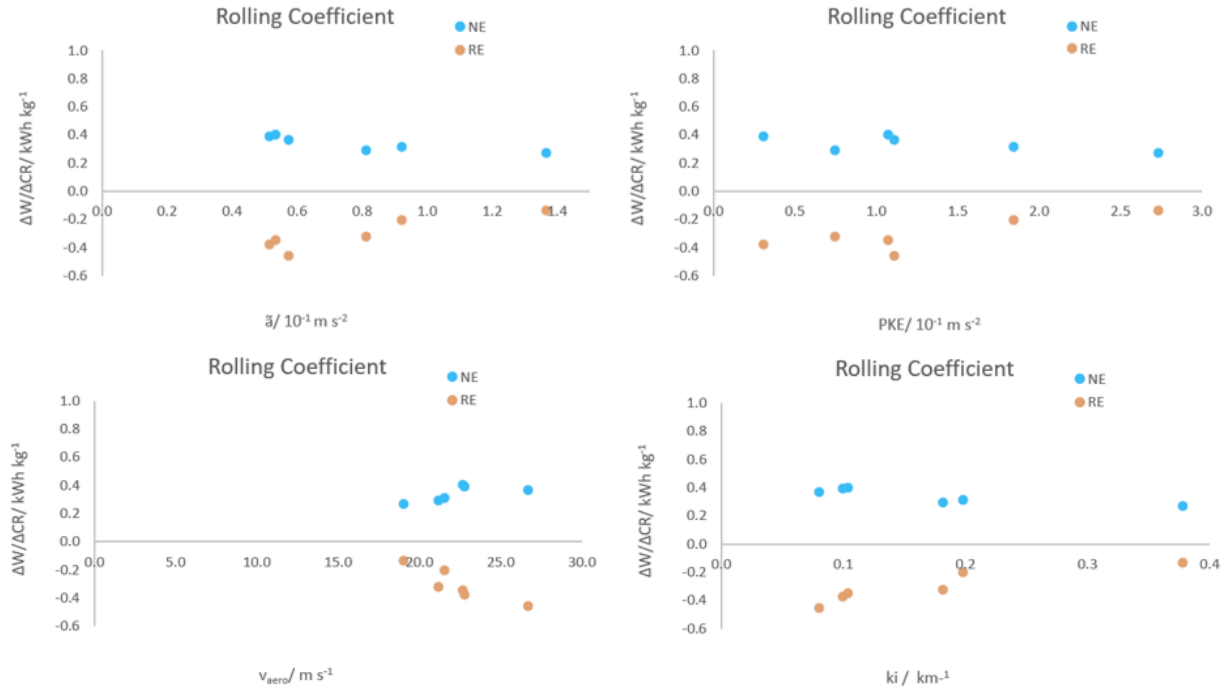


Figure G.5. Graphical representation of the relation between the energy variation and the vehicle rolling coefficient ($\Delta W/\Delta CR$) for different values of the cycle parameters: PKE , $\tilde{a}$, v_{aero} , and ki .

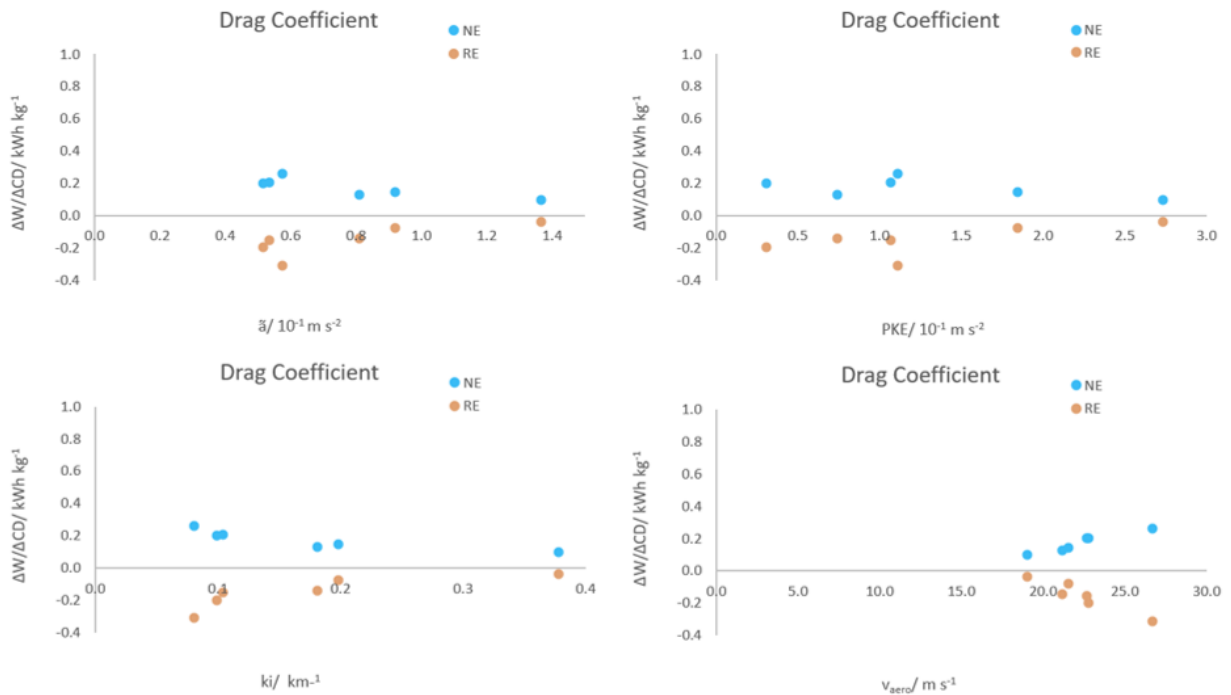


Figure G.6. Graphical representation of the relation between the energy variation and the vehicle drag coefficient ($\Delta W/\Delta CD$) for different values of the cycle parameters: PKE , $\tilde{a}$, v_{aero} , and ki .

Appendix H - Example properties

In order to simulate a representative example, the simulator assumed the HHDDT drive cycle, the vehicle properties defined in Appendix A -, and the FC and battery properties values displayed in Table H.1. The value of 0.12 for the A_{FC} was defined considering an internal project at DLR.

Table H.1. FC and battery properties defined for the representative example simulation.

Property	Value
$\alpha_+ / \text{A m}^{-2} \text{s}^{-1}$	220
$\alpha_- / \text{A m}^{-2} \text{s}^{-1}$	160
A_{FC} / m^2	0.12
$NC / (-)$	250
Battery capacity/ A s	93 600

Appendix I - Current and potential evolution

The simulator allows the user to observe the current density and the potential cell evolution along time as presented in Figure I.1

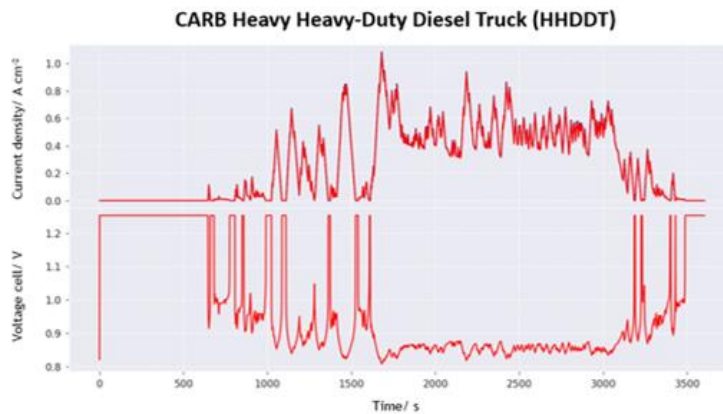


Figure I.1. Current density and cell potential evolution along time for the HHDDT cycle.

Comparing this plot with the drive cycle (Figure I.2) it is possible to understand that, when the speed increases, the current density is higher, and the potential is lower. This occurs since the cell potential is used to produce the current demand to achieve higher speed values.

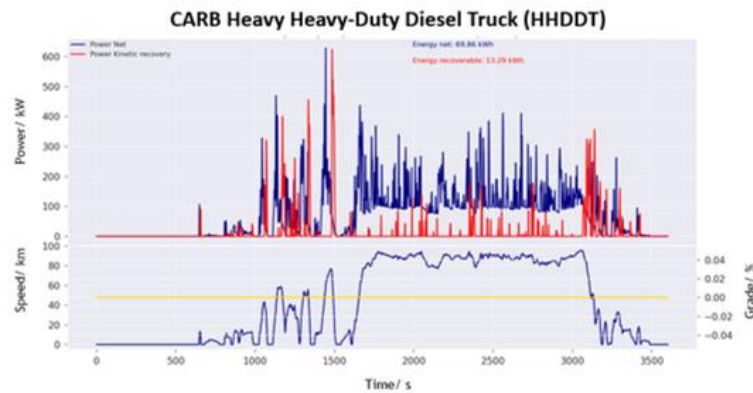


Figure I.2. $W_{NET,d}$ and $W_{kinetic}$ evolution over time, and respective drive cycle.

Appendix J - Operating conditions examples

In order to analyze three different operating conditions, the values established in Table J.1 were simulated. These values were selected considering an increase of 12 % in α_- between the examples (a) and (b) and a decrease of 12 % in α_+ between the examples (a) and (c).

Table J.1. Operating conditions for three different examples.

Property	Example (a)	Example (b)	Example (c)
$\alpha_+ / \text{A m}^{-2} \text{s}^{-1}$	250	250	220
$\alpha_- / \text{A m}^{-2} \text{s}^{-1}$	120	134	120
Battery capacity/ A s	93 600	93 600	93 600

After the simulation, it was possible to observe the SoC evolution for each example, as presented in Figure J.1.

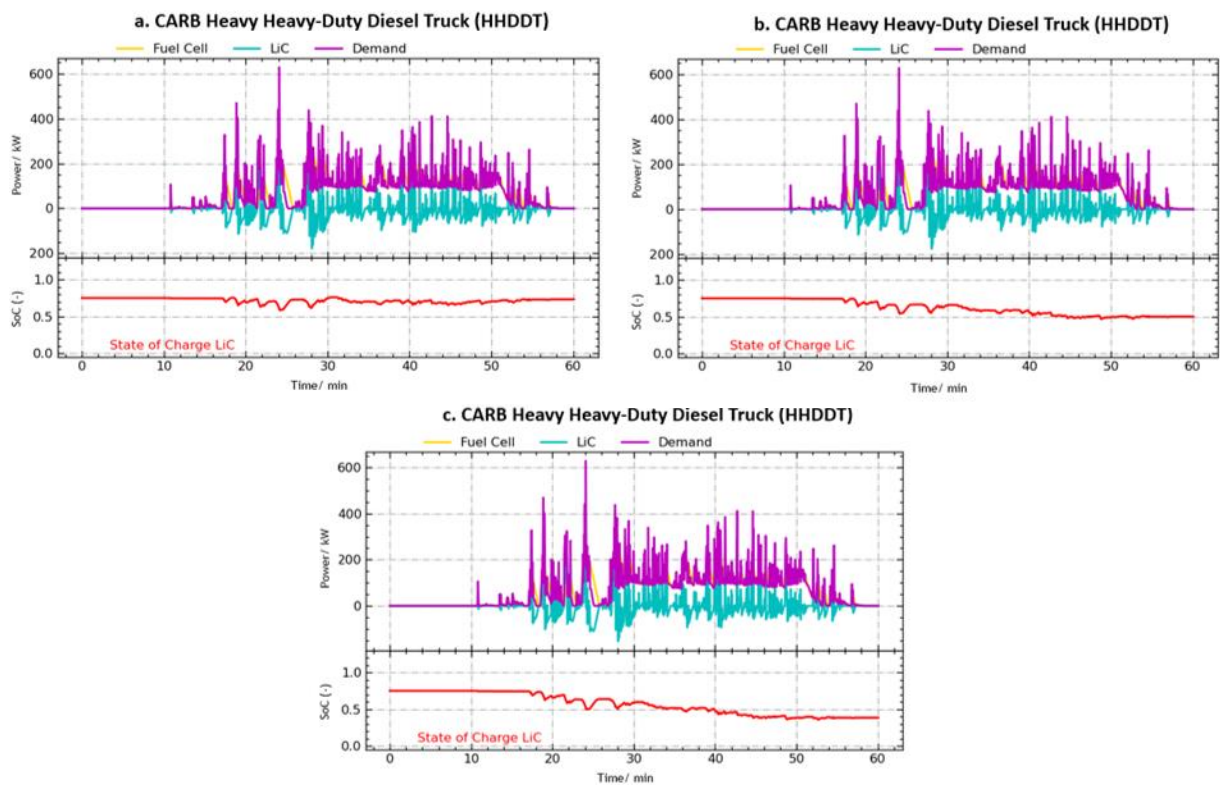


Figure J.1. Power and SoC evolution along time for three examples with different values of α_+ and α_- : $250 \text{ A m}^{-2} \text{s}^{-1}$ and $120 \text{ A m}^{-2} \text{s}^{-1}$ (a), $250 \text{ A m}^{-2} \text{s}^{-1}$ and $134 \text{ A m}^{-2} \text{s}^{-1}$ (b), $220 \text{ A m}^{-2} \text{s}^{-1}$ and $120 \text{ A m}^{-2} \text{s}^{-1}$ (c).

The SoC plots show that increasing α_- or decreasing α_+ , the battery achieves lower values of SoC since the current produced by the FC is lower. Also, it is possible to understand that a

similar variation in α_+ and α_- results in a slightly stronger SoC decrease for the α_+ variation example (c).

Regarding the FC power demand, the plots in Figure J.2 exhibit the results of each example under analysis.

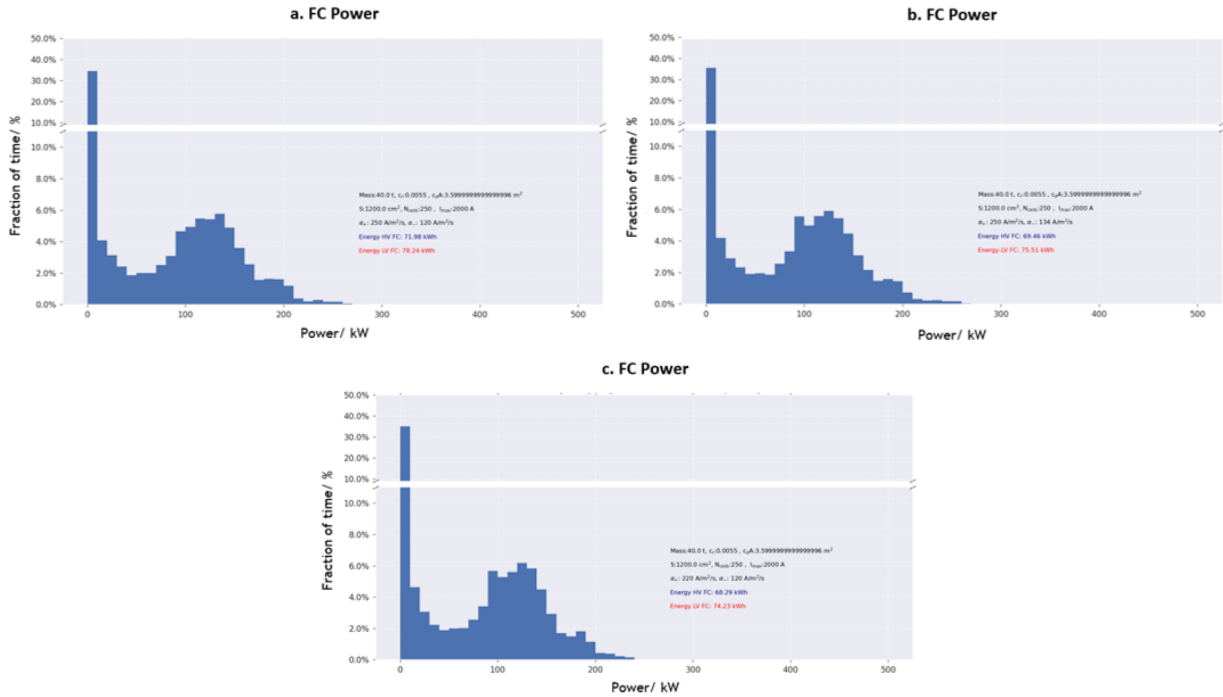


Figure J.2. Histogram with the drive cycle time spent in each FC power range for three examples with different values of α_+ and α_- : 250 A m⁻² s⁻¹ and 120 A m⁻² s⁻¹ (a), 250 A m⁻² s⁻¹ and 134 A m⁻² s⁻¹ (b), 220 A m⁻² s⁻¹ and 120 A m⁻² s⁻¹ (c).

The histograms analysis shows that in both situations the FC power demand displaces to lower values, which can be explained by the decrease in the FC current production in the examples.

On the other hand, the battery power demand histogram of each example does not show significant variations. Thus, changing 12 % of α_+ or α_- do not affect strongly the time fraction spent in each battery power range.

The time spent in each battery power range for the three different examples is displayed in Figure J.3. These plots show that in the three examples, the battery power distribution is similar.

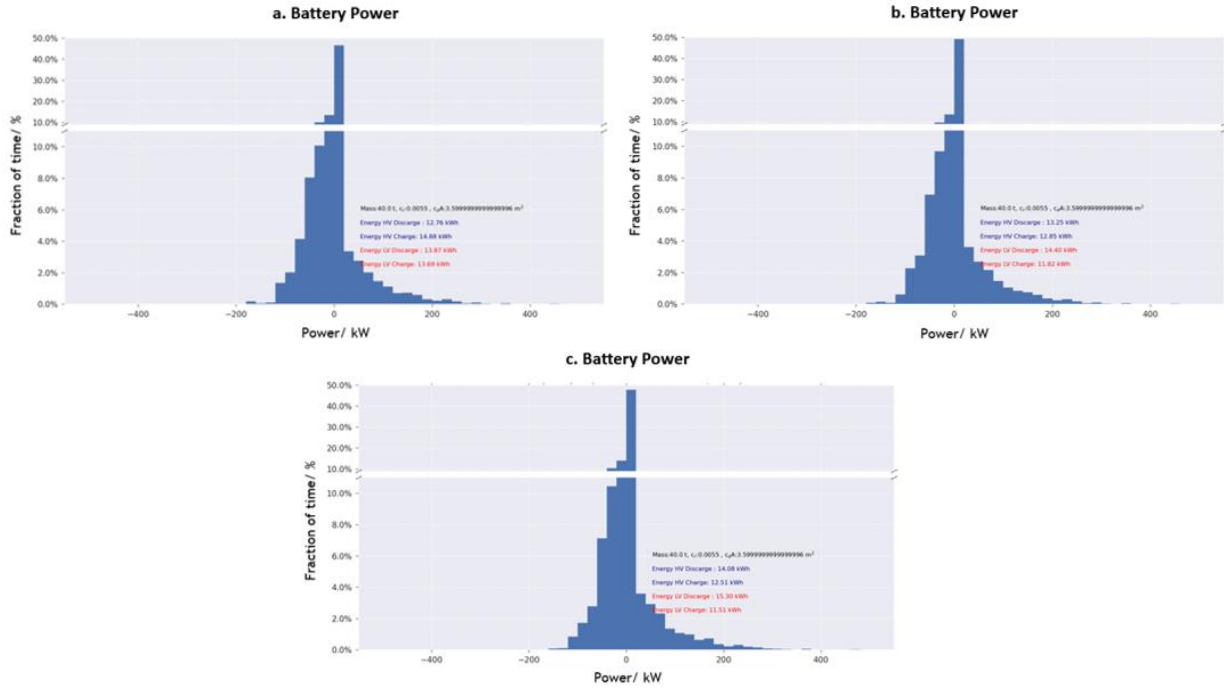


Figure J.3. Histogram with the drive cycle time spent in each battery power range for three examples with different values of α_+ and α_- : 250 A m⁻² s⁻¹ and 120 A m⁻² s⁻¹ (a), 250 A m⁻² s⁻¹ and 134 A m⁻² s⁻¹ (b), 220 A m⁻² s⁻¹ and 120 A m⁻² s⁻¹ (c).

The time spent in each system efficiency range for the three different examples is displayed in Figure J.4.

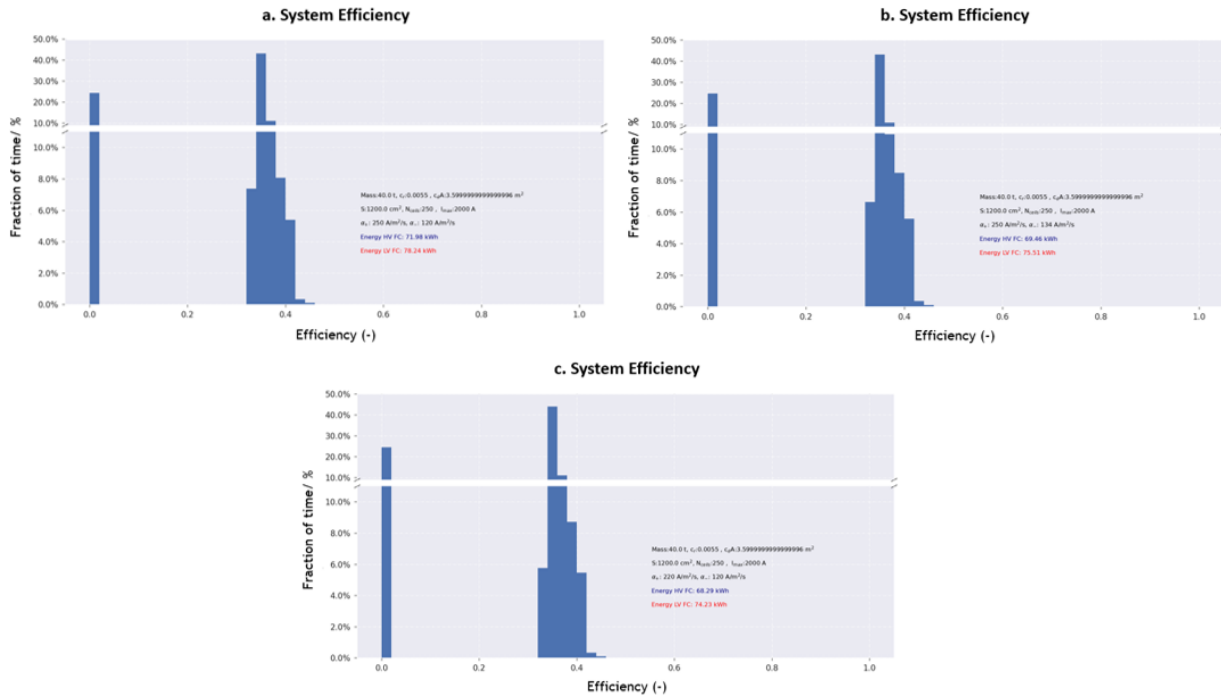


Figure J.4. Histogram with the drive cycle time spent in each system efficiency range for three examples with different values of α_+ and α_- : 250 A m⁻² s⁻¹ and 132 A m⁻² s⁻¹ (a), 250 A m⁻² s⁻¹ and 134 A m⁻² s⁻¹ (b), 220 A m⁻² s⁻¹ and 120 A m⁻² s⁻¹ (c).

The histograms show that increasing α_- or decreasing α_+ , the time spent in higher values of system efficiency increases.

Lastly, the $T_{min, rated}$ and H_2 consumption in each case is presented in Table J.2. It is possible to confirm that both the $T_{min, rated}$, and the H_2 consumption are lower for higher α_- and lower α_+ , when the FC produces lower current values.

Table J.2. $T_{min, rated}$ and H_2 consumption for three examples with different values of α_+ and α_- : a - (250 and 132) $A\ m^{-2}\ s^{-1}$, b - (250 and 160) $A\ m^{-2}\ s^{-1}$, c - (220 and 120) $A\ m^{-2}\ s^{-1}$.

Property	Example (a)	Example (b)	Example (c)
$T_{min, rated} / ^\circ C$	84.71	84.50	80.21
H_2 consumption/ g	5 477	5 277	5 178

Appendix K - Battery capacity influence

The variation of the battery capacity results in no significant differences for FC, BoP and global system efficiency, H_2 consumption, and $T_{\min, \text{rated}}$, as shown in Figure K.1 and Figure K.2.

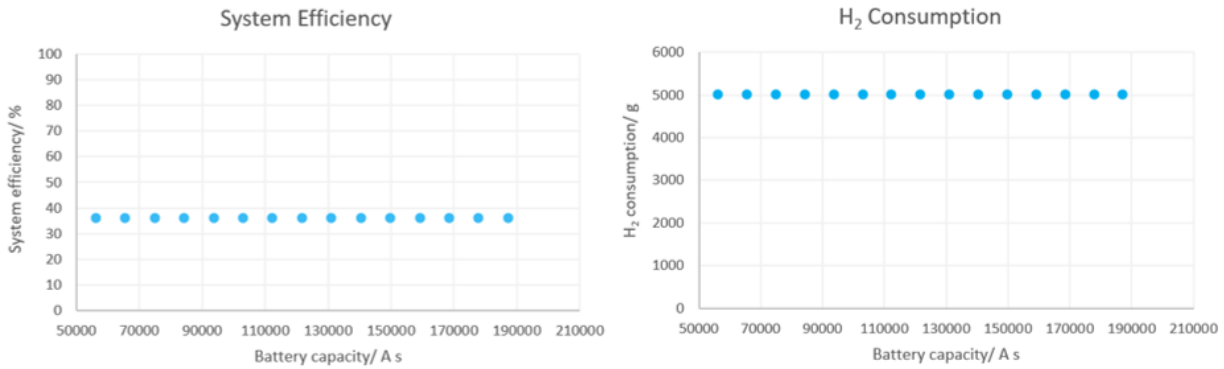


Figure K.1. System efficiency, and H_2 consumption for different values of battery capacity assuming constant α_+ and α_- as 230 and $140 \text{ A m}^{-2} \text{ s}^{-1}$, respectively.

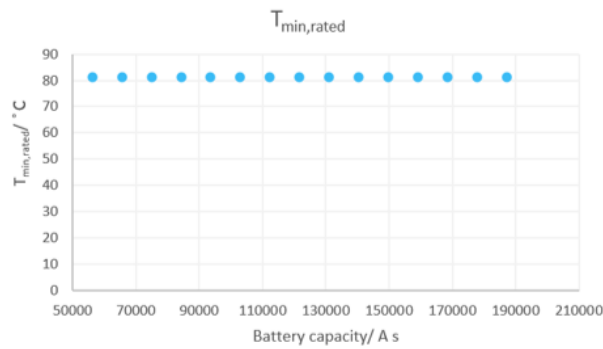


Figure K.2. $T_{\min, \text{rated}}$ for different values of battery capacity, assuming constant α_+ and α_- as 230 and $140 \text{ A m}^{-2} \text{ s}^{-1}$, respectively.