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Electrical Implementations of an Empirical Electrolyser Model for Improved Matlab/Simulink Simulations

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Abstract- Empirical electrical electrolyser models have proven to be effective in simplifying the analysis of multiple systems involving electrolyser. However, the conventional representation of current as an input of the electrolyser model present challenges for circuits involving power converters specifically in Matlab/Simulink implementations. This work presents an alternative representation of one of such models, using Lambert W function to use voltage as the independent variable. The function is implemented by using lookup tables to overcome slow calculations and algebraic loop errors. After validating the accuracy of the new representation against referred publications, a basic circuit using a non-isolated DC/DC boost converter is implemented to compare the performance of the conventional electrolyser model and the new representation. The simulation results show that the proposed representation not only works successfully in such systems, but also improves the simulation time up to 13% while fixing the inherent limitations of the conventional electrolyser model.

Keywords Electrolyser, Lambert W, Matlab/Simulink, DC/DC converter, Power converter.

1. Introduction

Hydrogen generation from water through electrolysers is a clean and sustainable alternative for energy requirements [1-5]. Designing, evaluating and improving renewable systems that utilize this technology requires modelling and simulation techniques to accomplish the desirable goal of each application.

The study of renewable energy systems integrated with hydrogen technology started back in 1980 primarily with alkaline electrolysers and solar panels. Most of publications have focused on connecting directly the electrolysers to the energy source as an alternative to simplify the overall system. This trend peaked on 2014 and may have started falling due to the inherent sacrifice in efficiency [2]. To improve the overall efficiency, power converters are usually deployed either to extract the maximum power available of the source or to regulate the electrical signals delivered to the load [6-7].

In terms of the electrolyser itself, several water electrolyser models have been proposed to either estimate the different parameters of the model or to implement the overall systems of equations that describe the system [8-10]. Due to their simplicity, empirical models are best suited for large systems analysis and specifically the one developed by Ulleberg has shown great level of accuracy and flexibility in representing different types of electrolysers [8, 11-14].

A Matlab / simscape / powersystems / Specialized technology model was presented by this author in [15] where the standard description of voltage given as a function of current was extended with boundary conditions to include transient responses on the electrolysers. However, if the model is used with power converters, MATLAB solvers require the handling of multiple algebraic loops which generates inconsistencies in the overall response of the electrolyser.

Previous studies have avoided the algebraic loops by removing the switching elements on the resulting electrical circuit or by using Simulink signals instead of electrical connections [16-17]. However, considering all the elements of the system in the electrical domain is essential for assessing the electrical behaviour of the resulting circuit.

To obtain a reliable electrical response of the electrolyser model, this work will present a variation of the model presented in [15], where the current is defined as function of voltage using lambert W prodlog function. The contributions of the proposed model are as follows:

- Resolve the existing limitations of the selected empirical model.
- Reduce the complexity of the model implementation in the MATLAB/Simulink environment.
- Allow smooth simulation results without removing switching elements or electrical components.
- Validate the accuracy of the electrolyser model against known data.

Initially the original model is presented highlighting its disadvantages. Next the new representation of the model is introduced and validated using data from two previous publications. Finally, a MATLAB/Simulink implementation is presented with a basic switching application to show the improvements with the proposed representation.

2. Electrolyser Electrical Model

The chemical process of water electrolysis separates a water molecule into its two constituent elements by applying energy in the form of electricity. This electrochemical process is temperature and pressure dependant and changes substantially depending on the type of ionic transport media or electrolyte. This electrolyte classifies an electrolyser in either alkaline, proton exchange membrane (PEM) or solid oxide (SOE). The full chemical description can be found in [8,18-19].

The design of the electrolytic cell, including electrodes materials, gap space, form, etc, change the response of the electrolyser even within the same type of electrolysers. Therefore, a model that can cover all the different variables providing a reliable response is a topic of constant research [8].

Among the many alternatives to electrolyser modelling, a simple solution is to utilize polarization curves of a real device and fit a given curve in terms of a small set of parameters. The one proposed in [20] takes six parameters to describe voltage as a function of current and temperature in the form of a logarithmic curve given by Eq. (1):

$$V_{elec} = N_c \begin{bmatrix} V_{rev} + (r_1 + r_2 T)\frac{I_{elec}}{A} + \\ s\log\left(\left(t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}\right)\frac{I_{elec}}{A} + 1\right) \end{bmatrix} \quad (1)$$

where: *T* is the temperature of the cell, *A* is the area of the electrodes, *Vrev* is the reversible voltage of the cell, *Nc* is the number of cells in series and *r1, r2, t1, t2, t3*, and *s* are the fitting parameters also known as overvoltage parameters. At standard conditions (1 bar, 25 ºC), *Vrev* is approximated to 1.229 V and can be considered constant for low temperature ranges up to 100 ^{0}C [20].

For many applications, Eq. (1) provides an accurate representation of the electrical response of the electrolyser providing reliable simulation outcomes [11]. In some cases, however, adjustments are needed to overcome the following issues:

- If current is equal to zero, Eq. (1) reduces the electrolyser to a dc voltage source which can supply energy to an external circuit.
- When electrolyser current is low, the term inside the logarithm can be negative producing complex values.
- In Eq. (1), any small current can generate a voltage. However, the chemical reaction only occurs after the external applied voltage is greater than the reversible voltage. Below this limit no current should be flowing through the electrolyser.
- Implementing electrical models in Matlab/Simulink, such as the one represented in Eq. (1), results in the creation of an algebraic loop that poses difficulties to the software solvers. Resolving these loops can cause distortions in the expected response of the model.

A proposed way to solve these issues was published in [15] where a set of boundary conditions are included to Eq. (1) to guarantee valid values regardless of the behaviour of the external circuit. The implementation in Matlab/Simulink, shown in Fig. 1, includes a diode that restricts current to flow only when the applied voltage is above the limit value of *NcVrev*. The algebraic loop was resolved with a memory block that works as a sample unit delay.

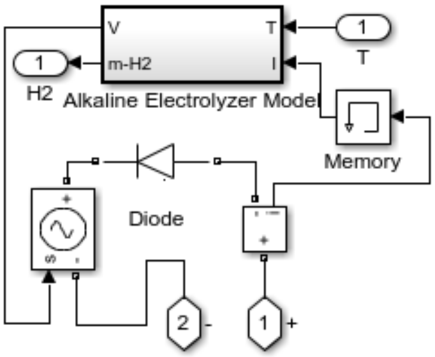


Fig. 1. Electrolyser simscape power systems block [15].

For simple circuits of few interconnected elements, this implementation is enough to obtain valid results. However, when the complexity of the system increases the expected outcome of the electrolyser model is heavily distorted. As a novel alternative, Eq. (1) can be changed to be a function of voltage instead of current, which allows the possibility to define the electrolyser operation in terms of the external applied voltage.

3. New model representation

3.1. Voltage as the domain of the function

Eq. (1) can be solved with respect to current using the prodlog or W Lambert function [21-22]. The steps shown below can be applied to any other model using logarithm functions.

First, the equation is rearranged, and some terms are renamed to simplify the visualization of the steps:

$$\frac{V_{elec}}{N_c} - V_{rev} = (r_1 + r_2T)\frac{I_{elec}}{A} + s\log\left(\left(t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}\right)\frac{I_{elec}}{A} + 1\right) \tag{2}$$

$$a = bI_{elec} + \log(cI_{elec} + 1) \tag{3}$$

Where,

$a = \frac{1}{s}\left(\frac{V_{elec}}{N_c} - V_{rev}\right)$, $b = \frac{1}{sA}(r_1 + r_2T)$, $c = \frac{1}{A}\left(t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}\right)$

Taking power of ten to both sides of Eq.(3), rearranging and renaming:

$$10^{a - bI_{elec}} = cI_{elec} + 1 \tag{4}$$

$$10^{-bI_{elec}} = \frac{c}{10^a}I_{elec} + \frac{1}{10^a} \tag{5}$$

$$10^{-bI_{elec}} = c'I_{elec} + d' \tag{6}$$

Where,

$$c' = \frac{c}{10^a} = \frac{1}{A10^{\frac{1}{s}\left(\frac{V_{elec}}{N_c} - V_{rev}\right)}}\left(t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}\right)$$

and $d' = \frac{1}{10^a} = \frac{1}{10^{\frac{1}{s}\left(\frac{V_{elec}}{N_c} - V_{rev}\right)}}$

Substituting $I_{elec} = \frac{t}{b} - \frac{d'}{c'}$ on Eq.(6):

$$10^{-t + b\frac{d'}{c'}} = \frac{c'}{b}t - d' + d' \tag{7}$$

$$\frac{b}{c'}10^{b\frac{d'}{c'}} = t10^t \tag{8}$$

Using Lambert function definition $xq^x = n \rightarrow x = \frac{W(n\ln q)}{\ln q}$ on Eq.(8):

$$\frac{W\left(\frac{b}{c'}10^{b\frac{d'}{c'}}\ln 10\right)}{\ln 10} = t \tag{9}$$

Back substitution $I_{elec} = \frac{t}{b} - \frac{d'}{c'}$ or $t = bI_{elec} + b\frac{d'}{c'}$

$$\frac{W\left(\frac{b}{c'}10^{b\frac{d'}{c'}}\ln 10\right)}{b\ln 10} - \frac{d'}{c'} = I_{elec} \tag{10}$$

Returning b, c' and d' terms back to the original form:

$$\frac{W\left(10^{\frac{(r_1+r_2T)}{s\left(t_1+\frac{t_2}{T}+\frac{t_3}{T^2}\right)}}\ln 10\frac{(r_1 + r_2T)}{s\left(t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}\right)}10^{\frac{1}{s}\left(\frac{V_{elec}}{N_c} - V_{rev}\right)}\right)}{\frac{1}{sA}(r_1 + r_2T)\ln 10} - \frac{A}{\left(t_1 + \frac{t_2}{T} + \frac{t_3}{T^2}\right)} = I_{elec} \tag{11}$$

To complete the electrolyser model, the domain of the function is defined for specific ranges of operation. For real values of voltage, the W function has two solutions or branches in the interval $-\frac{1}{e} \leq x < 0$ as shown in Fig. 2. For this application, the principal branch $-1 \leq W(x)$ satisfies the model.

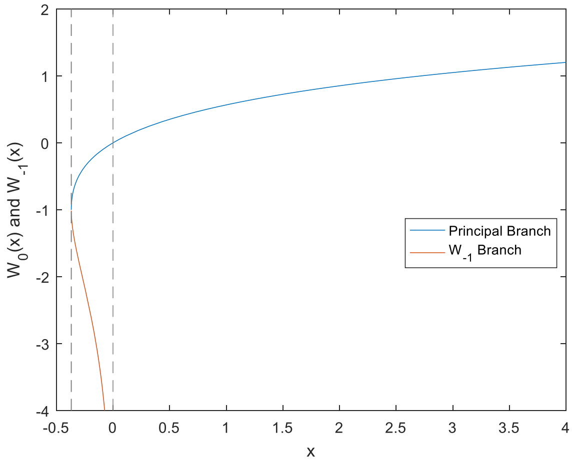


Fig. 2. Two main branches of the lambert W function [23].

Furthermore, to avoid the issues highlighted in the previous section, the voltage range is limited from 0 to N_cV_{rev} when there is no chemical reaction thus no current; and greater to N_cV_{rev} when the reaction is active and current passes through the electrolyser. The final electrolyser model with respect to voltage and temperature can be written as in Eq.(12).

The hydrogen production model remains unchanged and is rewritten from [15] in Eq.(13) where $\dot{M}H_2$ is the mass rate of hydrogen gas in kg per second, f_1 and f_2 are parameters related to Faraday efficiency, z is the number of electrons transferred in the reaction (2 electrons for water electrolysis), F is Faraday constant, c is a conversion constant equal to 0.08988 kg/m3 ; and v_{std} is the volume of an ideal gas at standard conditions 0.0224136 m^3/mol.

$$I=\begin{cases} 0 & 0<V<N_c V_{rev} \\ \dfrac{W\left(10^{\frac{(r_1+r_2T)}{s\left(t_1+\frac{t_2}{T}+\frac{t_3}{T^2}\right)}} ln10\,\dfrac{(r_1+r_2T)}{s\left(t_1+\frac{t_2}{T}+\frac{t_3}{T^2}\right)}10^{\frac{1}{s}\left(\frac{V_{elec}}{N_c}-V_{rev}\right)}\right)}{\frac{1}{sA}(r_1+r_2T)\,ln10}-\dfrac{A}{\left(t_1+\frac{t_2}{T}+\frac{t_3}{T^2}\right)} & V>N_c V_{rev} \end{cases} \tag{12}$$

$$\dot{M}H_2=\begin{cases} \left(\dfrac{(I/A)^2}{f_1+\left(\frac{I}{A}\right)^2}f_2\right)\dfrac{I}{zF}cv_{std}, & V>V_{rev} \\ 0, & V\leq V_{rev} \end{cases} \tag{13}$$

Table 1. Electrolyser fitting parameters

Electro-lyser	***Model parameters***						***Goodness of fit from curve fitting tool***			
	r1	***r2***	***s***	***t1***	***t2***	***t3***	***SSE***	***R-sqr***	***A-R-sqr***	***RMSE***
Alkaline	1.969e-4	-5.754e-7	0.1862	0.008887	-21.46	2362	3.402e-4	0.9989	0.9987	0.002781
PEM	2.379e-5	-1.13e-8	0.05518	0.7831	548.3	4335	0.00836	0.9989	0.9987	0.01866

3.2. Model construction and validation of the new representation

As previously mentioned, the process starts by finding the polarization curves of the devices to be modelled. Two electrolysers from published studies [20,24] are used as reference. Ten points are used to estimate the set of parameters for Eq. (1) using Matlab curve fitting tool. The list of final parameters is presented in Table 1 and a visual comparison between the reference and the model is shown in Figure 3.

To assess the new representation, the data points of the reference voltage for the two electrolysers are used as input of Eq. (12) and the results are compared to the reference current using the normalized root mean square error (NRMSE). This measure of differences is described by Eq. (14) and is useful when the comparison involves different scales. A result closer to 1 indicates a good fit. The results are presented in Table 2 and a visual comparison is shown in Figure 4.

$$NRMSE=1-\frac{\sqrt{\sum_{k=1}^{N}\left(y_{ref-k}-y_k\right)^2}}{\sqrt{\sum_{k=1}^{N}\left(y_{ref-k}-\overline{y_{ref}}\right)^2}} \tag{14}$$

Table 2. Electrolyser fitting parameters

	Alkaline	***PEM***
NRMSE 40 ⁰C	0.935666	0.977537
NRMSE 50 ⁰C	0.955586	-
NRMSE 60 ⁰C	0.951929	0.970202
NRMSE 70 ⁰C	0.980023	-
NRMSE 80 ⁰C	0.975527	0.971501
Data Points	10	10

3.3. Matlab implementation

The approach presented in [15] can be followed to implement Eq. (12) in Matlab/simscape/power systems/Specialized technology toolbox. However, the built in Matlab Lambert W function requires considerable computation time and is not practical for simulations that include multiple elements.

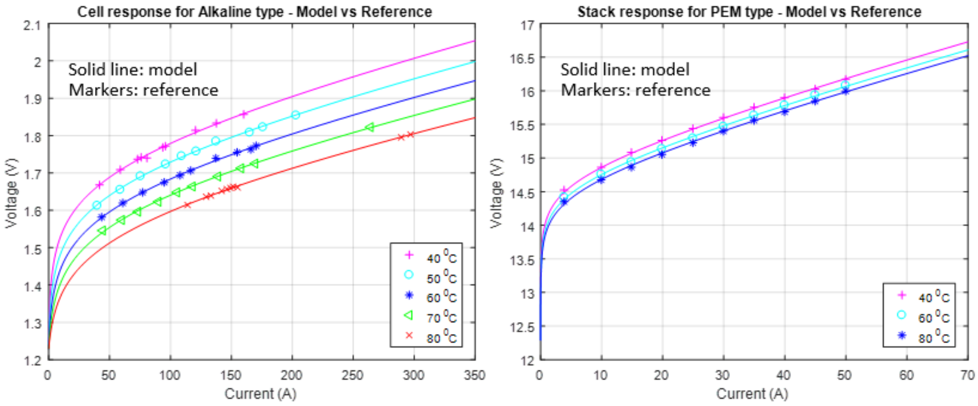


Fig. 3. Electrolysers electrical response, model vs reference

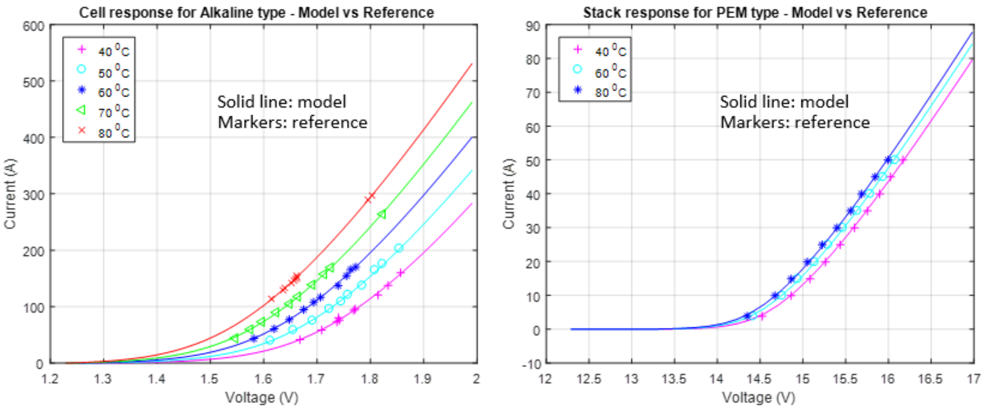


Fig. 4. New representation of the model vs reference.

To overcome the slow computational problem, a look up table is implemented where voltage and temperature are input variables and current is a matrix output generated by Eq. (12). The domain validation is now achieved with different switch selectors as shown in Fig. 5 and the diode is no longer required.

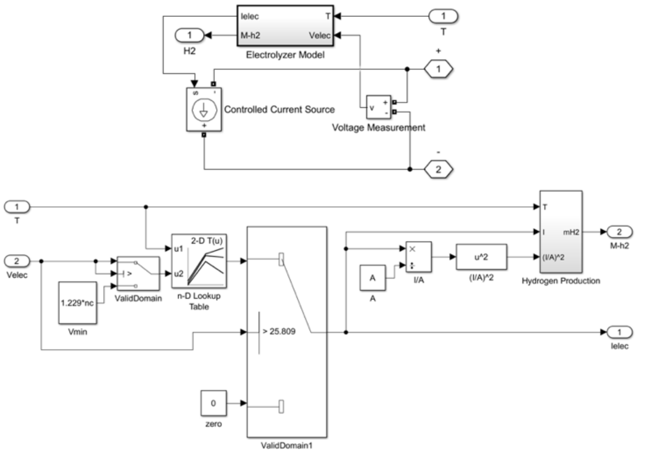


Fig. 5. Implementation of the New representation in Matlab/Simulink

The activation condition of the hydrogen production model in Eq. (13), is now implicit in the electrical current response of the new representation and allows a much simpler implementation as shown in Fig. 6.

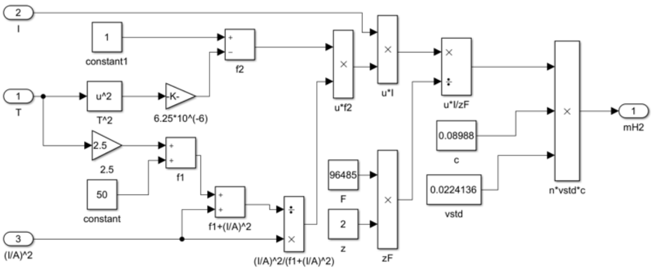


Fig. 6. Implementation of hydrogen production in Matlab/Simulink

To validate the implementation, the polarization curves of the electrolysers are generated using a controlled voltage source as shown in Fig. 7, and a numerical comparison between the reference and the model is calculated using the same technique as in the previous section. The results are shown in Fig. 8 and Table 3.

The integration method chosen is continuous mode to rely on the accuracy of the Simulink variable-step solver algorithms [25]. The Matlab recommendation for nonlinear models is followed by choosing Simulink solver ode23t mod. Stiff/Trapezoidal with default values [26]. A maximum step size of 1 x10^{-06} is chosen only for the circuit shown in Fig. 7

to get voltage values approximately close to the reference values and to obtain a meaningful comparison.

Table 2. Electrolyser fitting parameters

	Alkaline	*PEM*
NRMSE 40 ^{0}C	0.935664	0.977537
NRMSE 50 ^{0}C	0.955585	-
NRMSE 60 ^{0}C	0.951927	0.970202
NRMSE 70 ^{0}C	0.980025	-
NRMSE 80 ^{0}C	0.975527	0.971501
Data Points	10	10

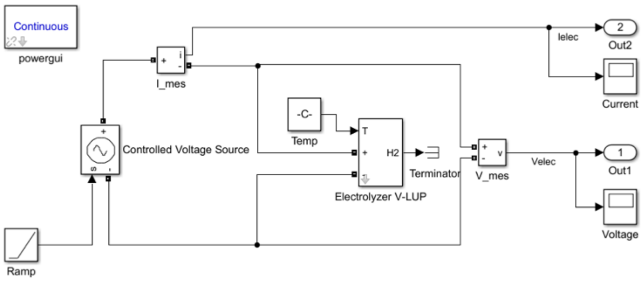


Fig. 7. Circuit to obtain polarization curves in Matlab/Simulink

4. Simulation of a switching application

To assess the benefits of the new representation, a system implementing a DC/DC boost converter feeding an electrolyser is developed as shown in Fig. 9. The input and output voltage values of the boost converter are arbitrarily defined to be 10 and 35 Volts, respectively. The duty cycle (D) required to achieve this conversion is found to be 0.7143 using equation (15) [27]. The values of inductance and capacitance are set to provide good filtering with a smooth response for a switching frequency of 10 kHz.

$$V_{out} = \frac{1}{1-D} V_{in} \tag{15}$$

The two electrolysers are approximately set up to the same range of operation by adjusting the number of cells. At 35 volts and temperature of 23 ^{0}C, the currents of a 21-cells-alkaline and a 23-cells-PEM electrolyser are found to be 13.8797 A and 14.6294 A, respectively. These values of voltage and current relate to an equivalent resistance of approx. 2.5 ohms.

The simulations total run time is 1 second and the switching is enabled after 0.3 seconds. The algebraic loop introduced by the electrical implementation is forced to be solved iteratively by Simulink algorithms to obtain high accuracy [28].

When the system uses the electrolyser conventional model, Simulink is unable to solve the loop for specific scenarios and therefore the following approaches are followed to obtain valid solutions:

- Introducing two common loop breaking techniques with either a unit delay block or a first order transfer function.
- Implementing a lookup table for the conventional model.

The unit delay approach was implemented in [15] with a memory block and is equivalent to a unit delay block. The first order transfer function uses the same form of a low pass filter and the time constant works as the cut-off frequency. With a switching frequency of 10 kHz, a time constant lower than 1.6 x10^{-5} is needed to at least cover the switching dynamics without harmonics. Unfortunately, the simulation time increases considerable as the time constant is reduced

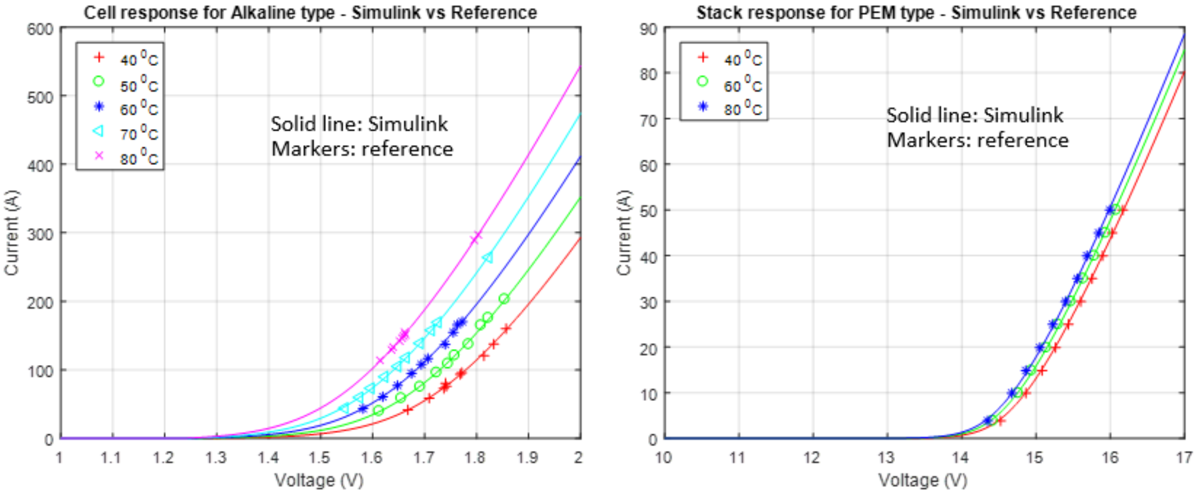


Fig. 8. New representation using simulink, model vs reference.

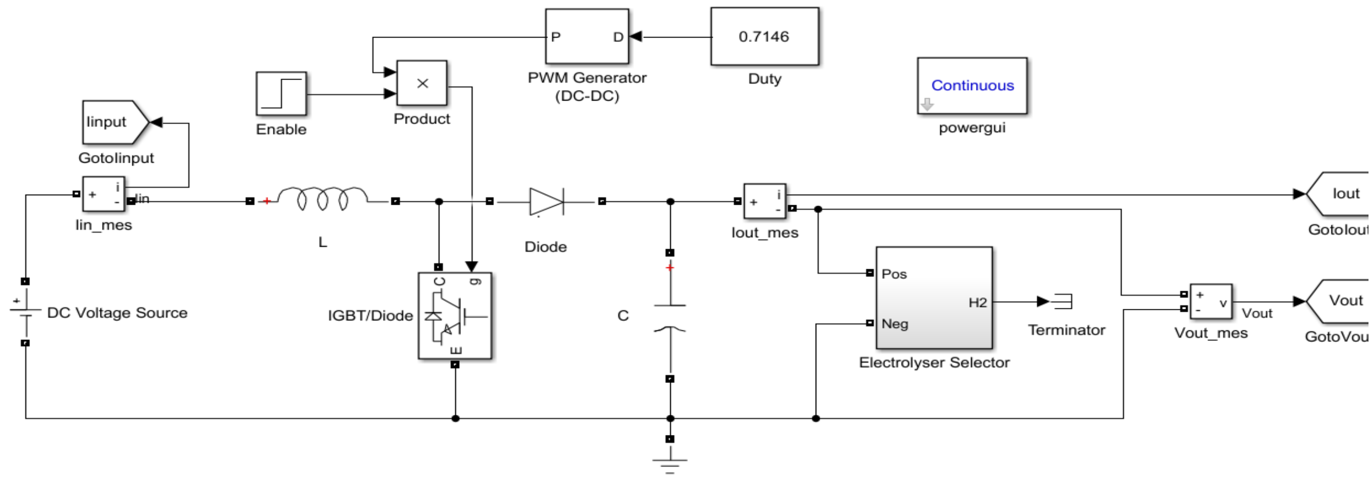


Fig. 9. Boost converter and electrolyser system.

and only a time constant of 1 x 10^{-5} is assessed.

A lookup table is constructed similarly as described in the previous section by creating a voltage output matrix using Eq. (1). The electrical implementation remains unchanged but instead of constructing Eq. (1) with Simulink blocks, a lookup table is introduced as shown in Fig. 10.

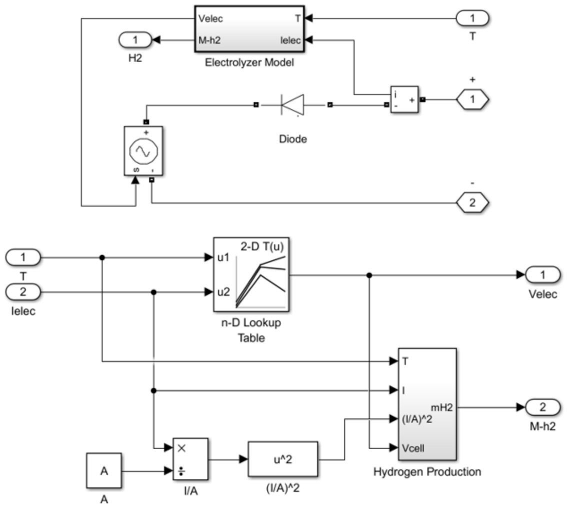


Fig. 10. Lookup table implementation for the conventional model

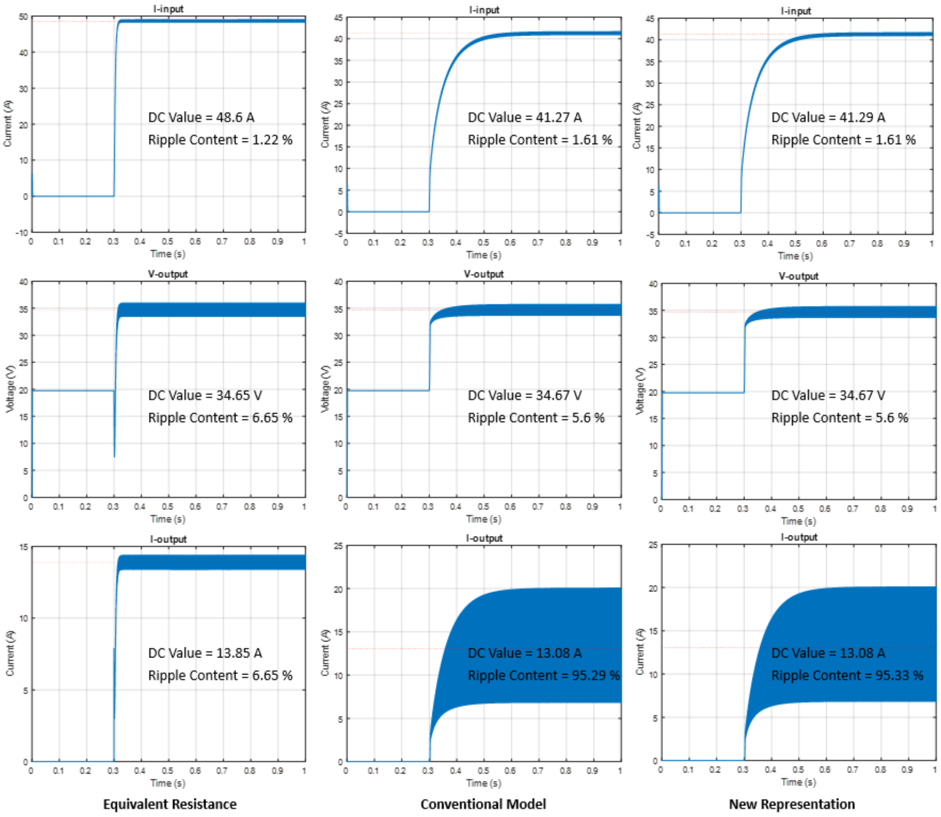
5. Results and discussions

The system is first tested using the equivalent resistance to assess the converter conversion and observe the overall results. With a filter capacitor of 400 µF, the linear load produces a ripple content of 6.65% in both output signals. The alkaline electrolyser is introduced next producing a degraded ripple content due to its non-linearity against small variations of voltage. For this scenario, Simulink can solve the loop for all models, showing equivalent results between them as shown in Fig. 11 and Table 3.

Table 3. Results with filter capacitor of 400 µF

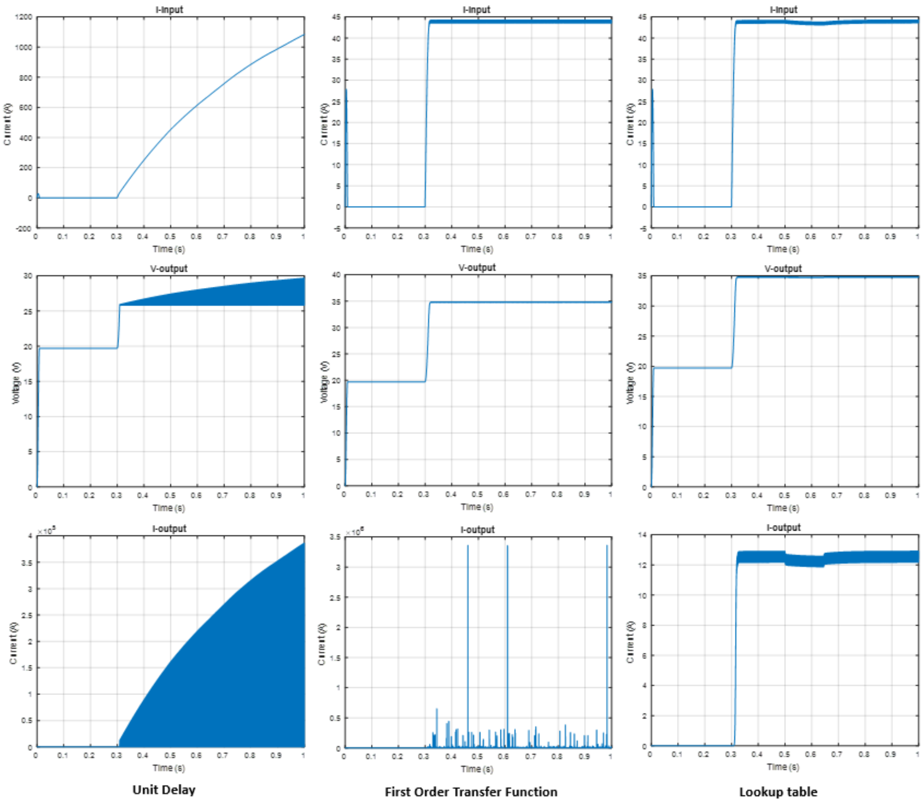
	Eq. Resistance		***Conventional***		***New Rep.***	
	DC	***Ripple %***	***DC***	***Ripple %***	***DC***	***Ripple %***
I_{in}	48.6 A	1.22	41.27 A	1.61	41.29 A	1.61
V_{out}	34.65 V	6.65	34.67 V	5.6	34.67 V	5.6
I_{out}	13.85V	6.65	13.08 A	95.29	13.08 A	95.33

To reduce the ripple content on the output signals the filter capacitor is increased to 8000 µF. Under this scenario, Simulink cannot solve the algebraic loop in the conventional model and the techniques described in the previous section are assessed to verify the best results.



Equivalent Resistance **Conventional Model** **New Representation**

Fig. 11. Simulation results for the system using 400 μF



Unit Delay **First Order Transfer Function** **Lookup table**

Fig. 12. Loop solving techniques results for the conventional model using 800 μF

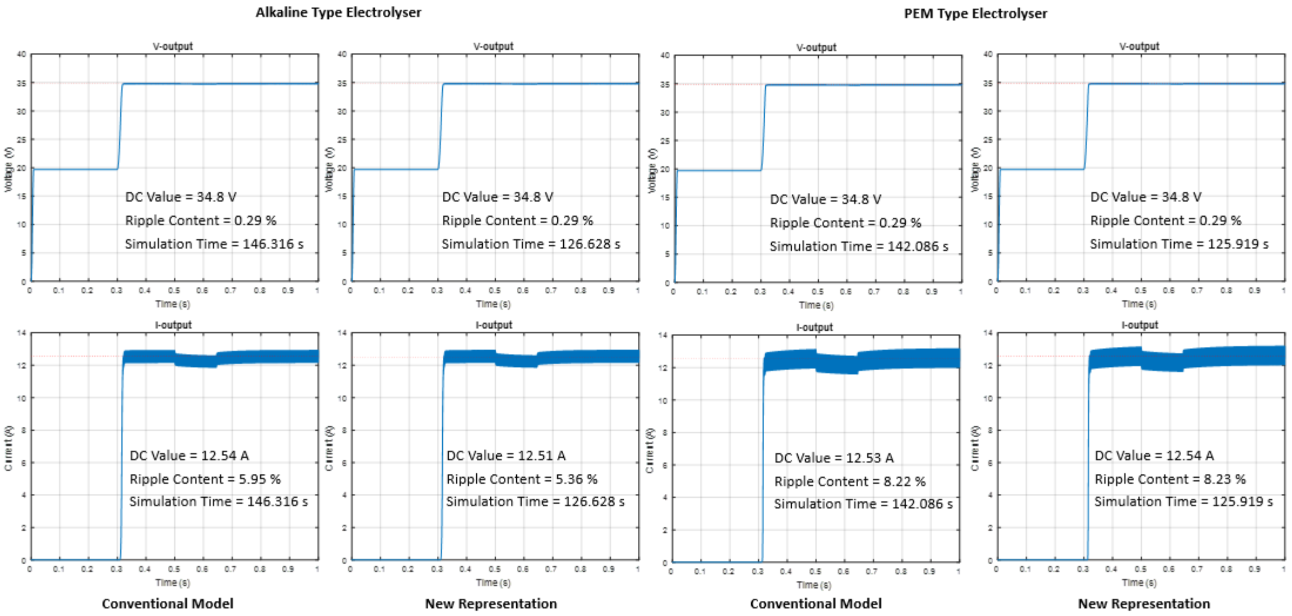


Fig. 13. Simulation results for two electrolyser types using different models

table implementation producing the results in Fig. 12. The controlled voltage source and the capacitor voltage of the conventional model dictates the input current which needs to vary to satisfy the circuit state equations. For a unit delay, the model never receives the correct value of current and ends up oscillating with a divergent amplitude. For a first order transfer function, the current oscillates to guarantee a correct voltage transition between the capacitor and the controlled voltage source. For the lookup table, the complexity of the model is reduced which allows Simulink to solve correctly the system of equations.

Finally, a comparison is performed between the new representation and the conventional model using the lookup table implementation for both models. Additional to the circuit metrics, total simulation time is added to the performance metrics to assess the best alternative. Simulations are run for the two electrolyser types, PEM and Alkaline using both models. The results presented in Fig. 13 and Table 4-5, show that the circuits metrics are equivalent with small discrepancies in the current signals. Simulation time is longer for the conventional model requiring approx. 13 % extra time than the new representation.

Table 4. Simulation results for alkaline type

	Conventional (146.316 s)		***New Representation (126.628 s)***	
	DC	***Ripple %***	***DC***	***Ripple %***
V_{out}	34.8 V	0.29	34.8 V	0.29
I_{out}	12.54 A	5.95	12.51 A	5.36

Table 5. Simulation results for PEM type

	Conventional (142.086 s)		***New Representation (125.919 s)***	
	DC	***Ripple %***	***DC***	***Ripple %***
V_{out}	34.8 V	0.29	34.8 V	0.29
I_{out}	12.53 A	8.22	12.54 A	8.23

6. Conclusion

A new representation of the electrolyser empirical model was presented to extend its application to larger electrical systems with several components. Lambert W function is used to change the form of the model to be voltage dependant, allowing a simpler implementation that results in an improvement of overall simulation time.

A Matlab/Simulink implementation using lookup tables is presented as a simplification approach to speed up the simulation and to allow recursive algebraic loop by the solver for greater accuracy. When running simulations for a system composed of a DC/DC boost converter and an electrolyser, the lookup table implementation shows an accurate result against the common loop handling techniques of a unit delay and a first order transfer function. In terms of model comparison, the new representation improves the total simulation time by 13%.

The analysis presented here can also be applied to other electrolyser models that may face similar challenges when interacting with multiple elements

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