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Direct methanol fuel cells: A database-driven design procedure

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ABSTRACT

To test the feasibility of DMFC systems in preliminary stages of the design process the design engineer can make use of heuristic models identifying the opportunity of DMFC systems in a specific application. In general these models are to generic and have a low accuracy. To improve the accuracy a second-order model is proposed in this paper. The second-order model consists of an evolutionary algorithm written in Mathematica, which selects a component-set satisfying the fuel-cell systems' performance requirements, places the components in 3D space and optimizes for volume. The results are presented as a 3D draft proposal together with a feasibility metric. To test the algorithm the design of DMFC system applied in the MP3 player is evaluated. The results show that volume and costs are an issue for the feasibility of the fuel-cell power-system applied in the MP3 player. The generated designs and the algorithm are evaluated and recommendations are given.

1. Introduction

In the past 10 years more portable electronics have entered our lives. All of these electronic devices are powered by a battery and mainly the rechargeable lithium ion battery. The market for portable electronic devices is increasing. Connectivity to the internet and more functionality makes these devices long for a longer run-time and higher power use [1–3]. To increase run-time a direct methanol fuel cell (DMFC) power system has a lot of potential due to its high energy dense fuel, methanol.

In [4] different tools and methods are described which can be used to design or select a power system for a specific application. In general a systematic approach is used to bring an idea, via specifications, conceptualization and embodiment to finally an engineered product. The identification tools like PowerQuest [5], the CES method [6,7] and working with Ragone plots [8,9] are based on normalized figures like energy density, and therefore not always correct. The numbers outputted from these programs cannot be used to evaluate concepts but merely identifies the opportunity. Improvement in these tools is needed giving more than just initiatives or making alternative power sources visible. Tools like T-max, developed at Jet Propulsion Lab [10,11], evaluate the power system instantly when changes in the design are made, are a must for the concurrent design engineer. Generalized and instant evaluation tools should be developed to give the designer improved basis for their concept choice.

To test the feasibility of DMFC systems applied in portable electronic devices during the preliminary design stages a first-order heuristic model is presented in Flipsen [4]. This model was based on a case-study by Motorola [12,13] and two design cases [14,15] the weight and volume of a DMFC system is calculated by breaking down the system into five major contributors: (i) the fuel cell stack, (ii) the balance of plant (BOP), (iii) the empty space, (iv) the intermediate accumulator and (v) the fuel tank. In Section 4 the first-order model is briefly evaluated by two commercially available DMFC power systems. The output of the model shows a wide range in the predicted system volumes, making the model low accurate.

To improve the first-order model the results' ranges should be narrowed down, making the model more accurate. This can be done by evaluating more commercially available DMFC systems. Due to the low amount of commercially available DFMC power systems, it is justified to use a more accurate, second-order model for optimization of the first-order model. This paper will elaborate further on the on the second-order model (Section 3). The second-order model is a database-driven algorithm which chooses and evaluates a set of commercially available components to be used in a low-power DMFC power systems. The algorithm is presented and implemented in a software program written in Mathematica. Based on the applications' load-profile the program chooses a component-set which suffices the fuel-cell systems' performance requirements. The placing of the chosen component-set is optimized for volume and a draft proposal together with a feasibility metric is presented to the designer. To test the algorithm the design of DMFC system applied in the MP3 player is evaluated (Section 4). The results are discussed and conclusions are drawn in Sections 5–7 on the feasibility of the power system and the algorithm is evaluated.

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2. Different orders of modeling

In this paper we define four orders of modeling, from basic comparison based tables and figures (zero order), through the heuristic approach (first order) to the automated design using algorithm (second and third order). The first two approaches use normalized equations and are to be used without the computer. The higher the order of modeling the higher the accuracy, but also the complexity. For higher order models the computer is used to evaluate multiple designs on one or more objectives. The second order model optimizes for 'basic' properties, while the third order model also includes other more 'specific' properties.

2.1. Zero order model: general comparison

In Flipsen [16] a comparison between power sources is made, based on normalized values for energy, power and costs. This type of model we like to call the 'zero order model' giving good indication what the overall opportunity is for a specific power system. Although power systems are made visible to the designer with simple comparing plots, this method does not identify an opportunity for a specific power source applied in a portable electronic device which exists or has 'to be designed'.

2.2. First order model: heuristic approach to modeling a DMFC power source

The next order model, the 'first order model', will help the designer in evaluating the feasibility of a power source (in our case the DMFC power system) in comparison with other power sources (in our case the lithium-ion battery). Based on a case-study by Motorola [12,13] and two design cases [14,15] the weight and volume of a DMFC system is calculated by breaking down the system into five major contributors: (i) the fuel cell stack, (ii) the balance of plant (BOP), (iii) the empty space, (iv) the intermediate accumulator and (v) the fuel tank. The first-order model gives good feedback to the designer whether a DMFC system is feasible and how large it will be. This type of modeling is generally used in conceptual design, and known as a "rule of thumb", where equations give the designer preliminary insight in a specific problem or identify opportunities for specific technologies. This type of modeling can best be used when no computer is available.

The input data in the model is moderate, but still needs knowledge of the designed or to be designed device. User profile is needed which is used to define a load profile. The designer has to know how high the load will be when the user uses a certain function. Development of the load profile in the form of a power-to-time function or graph is needed to give a good estimate of the DMFC hybrid physical performance. The designer has to fall back on its electronics knowledge and describe the power needed for every function of the application. Summing all power data for every function will give the designer insight in the potential power needs of the product. The model is presented in [4,14] and validated with two commercially available fuel cells systems produced by Smart Fuel Cell (SFC) [17]: the Jenny (25 W, 400 Wh) and the Efoy2200 (90 W, 5.5 kWh). The output of the model showed a wide range in the predicted system volumes, making the model too generic with a low accuracy. A more accurate approach is desired which is presented in this paper.

2.3. Second order model: database-driven metrics-based design

The first order model described in the previous section gives a quick impression of the feasibility of a DMFC power system applied in a portable electronic device. Problems with this model are the (i) accuracy of the model, (ii) the low amount of properties to optimize for, and (iii) the lack of a single metric, showing the product designer the improvement opportunity.

One part of design and engineering is the act of sizing, dimensioning and selecting the detailed elements of the design. This part of the design process can be used to test the feasibility of different design concepts, by using the computer to evaluate multiple design solutions on one or more parameters. In general the designer can only evaluate a limited amount of structural variants (often less than five) on a limited amount of objectives (often only volume), with a low amount of differentiating components. Within these structural variants there are variables which specify the main proportions, like weight, dimensions and costs, but also other details of the application. To test the feasibility of different concept design, and not only structural variants, a "quantified optimum design" method can be used. Quantified parameters are used to evaluate a concept with the help of the computer which can evaluate a greater deal of concepts in less time than a designer could.

For the second-order model the accuracy could be improved by evaluating multiple structural variants with the help of the computer. All structural variants are generated by the computer and are build up from standard building blocks (parallelepipeds), representing all basic components needed in a fuel-cell system. New metrics are introduced for all basic properties, and an objective function is defined with whom the design is evaluated by. In Section 3 the second order model is proposed using the computer to evaluate multiple structural variants and optimized for three basic properties: volume, price and weight. Components are chosen from a database consisting of geometrical and non-geometrical data.

3. Second order model

In this section a different approach is proposed to test the feasibility of a fuel cell system in a specific application. The approximation does not consist of a simple formula but evaluates multiple architectures, or structural variants. The evaluation is based on a multi-parametric optimization algorithm, where volume, weight and costs are the three basic properties.

In this section an introduction is given on preference-based optimization, followed by an explanation of all metrics which will be optimized for. To facilitate understanding, comparison and weighing of the effect of different properties, all properties are made dimensionless. The dimensionless properties are called metrics M appropriately and are not all equally important. The importance of the metric is defined by the preference factor λ, and the values are based on the values found in [18]. Multiplying the dimensionless factors with the specific preference factors gives the function $F(D)$ to optimize for. The optimization function is applied in the design algorithm proposed in Section 3.9. The optimization function is used to find the most optimized architecture of a DMFC system applied in a specific application. The algorithm presented is evaluated by applying it to the design of a DMFC system for the Samsung YP-Z5F MP3 player.

3.1. "Automated design" approach

The approach proposed in this section is a numerical evaluation of multiple structural variants optimized for a single objective consisting of different dimensionless metrics. The computer is used to do more than merely analyze engineering designs, but also makes design decisions and lead the design to an improved solution, in short an "automated design" approach. In this automated design process an optimization algorithm is used to optimize the system for the basic metrics. In literature the approach for optimized layout design is used in aeronautical environments, where the 3D packing problem with performance constraints is generally impossible to

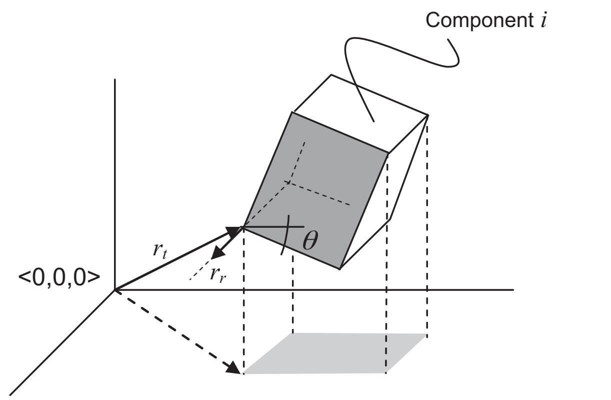

Fig. 1. Definition of the translation vector r_t, the rotation vector r_r and the rotation angle θ for a specific component i.

solve only by engineers experience and intuition [19,20], but also in the design of circuit boards and IC chip layout [21] and loading of ships, trucks and trains [22].

3.2. Design variables

The numerical quantities for which values are to be chosen in producing the design will be called "design variables" [23]. For the DMFC system the position in space and rotation of the different components are design variables. Amongst other properties we want to minimize volume of the total design by changing these variables. All design variables can be combined in a *Design vectorD*, which simply is a list containing all the design variables for a particular problem. For the case study the only design variables used to define a solution is the placing of components in space:

$$\vec{D} = \left((\vec{r}_t, \vec{r}_r, \theta)_1, \ldots, (\vec{r}_t, \vec{r}_r, \theta)_i\right), \text{ for } i = 1, 2 \ldots n \quad (1)$$

where r_t, r_r and θ are the translation vector, the rotation vector around which the object will rotate about, and the angle to rotate respectively for all n objects in the design. The objects in the design are components, amongst others the fuel cell, fuel tank and pumps. Every combination of these variables refers to a specific architecture or placing of objects related to each other in space (Fig. 1).

3.3. Design constraints

At this point a design is now simply a set of values of design variables defined by the design vector D. It must be noted that the size of the components are taken from a database of components which are chosen based on their performance specifications (see Sections 5 and 5.3). To produce an acceptable design restrictions are introduced, further called the "design constraints". There are three categories of constraints: side constraints, behavior constraints and constraints arising from a discrete-valued design variable [23].

A constraint restricting the range of design variables for other than the direct consideration of performance is called a *side constraint*. In our design example a side constraint is amongst others the systems length that should be in between a minimum and maximum:

$$g(D) = 0.5 l_{battery} \leq l_{system} \leq 1.5 l_{battey} \quad (2)$$

In the above example the minimum and maximums systems length is related to the benchmarked value used in the application, in our case the length of the battery.

A constraint derived from the performance or behavioral requirements is called *behavioral constraint*. A behavior related constraint is in our case amongst others the design of the fuel tank which is related to the energy E needed in the application:

$$h(D) = l_t h_t w_t = E(u\rho)_{fuel} \quad (3)$$

A *discrete-value constraint* is a constraint which arises when the design variable is not selected from a continuous range of values but is permitted to take only one of discrete values. In our case the rotation angle is constrained to rotations in quantities of $1/2\pi$:

$$j(D) \equiv \theta = k\frac{1}{2}\pi, \text{ with } k \in Z \quad (4)$$

3.4. The objective function

In general the goal of multi-objective optimization is to find a set of solutions as close as possible to the Pareto optimal front, Fig. 2 [24]. This means there is more than one optimal solution (which is always the case) to the multi-objective optimization problem. In Fig. 2 an optimized Pareto front is created by changing the preference factor λ_i for both the optimized functions, or the objectives, f_1 and f_2, where $f_i = \lambda_i M_i$. The gradient of the lines in the figure describe the importance of the different optimized functions. By changing the preference factors the Pareto optimal front is created. A change in the preference factors will result in a different optimal solution. The factors should therefore not be arbitrarily chosen. To find the best trade-off the results from the conjoint analyses are used to produce the best set of preferences.

Preference bases multi-objective optimization is often used to simplify a problem to a single objective optimization problem, resulting in a single solution, the *combined optimization function*. The method used in this work is called the Weighted Sum method [24], which scalarizes a set of metrics into a single objective function $F(D)$ by pre-multiplying each metric $M_i(D)$ with a user-supplied weight λ_i:

$$\min \; F(D) = \sum_{i=1}^{m} \lambda_i M_i(D) \quad (5)$$

All metrics used have to be handled and converted in the same type, a maximizing or minimizing metric. The object metrics in our case are all of the minimizing type: minimizing volume, minimizing weight and minimizing costs. Dimensional unit effects are taken out of the picture by making all metrics dimensionless, resulting in normalized metrics M_i.

3.5. Explanation of metrics

Following this procedure of the weighted sum method, the metrics used have to be defined. Three basic properties are proposed for

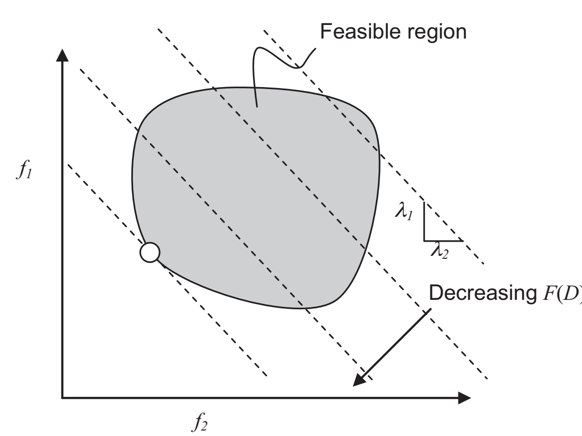

Fig. 2. The weighted sum approach for a convex objective space.

use in the second-order model: volume, weight and costs. To sum the minimizing properties to each other we have to make them similar in dimension. To do this the properties are normalized to the specifications of the benchmarked power source used in the application. This means the calculated costs for the DMFC power system is divided by the costs of the benchmarked lithium polymer battery:

$$M_C = \frac{C_{fc-system}}{C_{accu}} \tag{6}$$

The same thing can be done with the other two basic properties:

$$M_m = \frac{m_{fc-system}}{m_{accu}} \tag{7}$$

And:

$$M_V = \frac{V_{fc-system}}{V_{accu}} \tag{8}$$

Weight and dimensions are taken from specifications sheets for all components. To make an assumption for the "purchase price" the costs for the benchmarked power source and all components used in the fuel cell system are set at a price per piece when purchasing 100 pieces.

3.6. Relative preference factor λ

The optimization function depends on three metrics defined in the previous section. It is impossible to find the optimum in which all metrics are minimized, making a trade-off necessary. Because some metrics are more important than the others, the preference factor λ_i is introduced. The preference factor gives the importance of the specified metric compared to the other metrics. All preference factors summed together must be equal to 1:

$$\sum_{i=1}^{m} \lambda_i = \lambda_1 + \lambda_2 + \ldots + \lambda_m = 1 \tag{9}$$

Based on higher-level information, the preference factor is first chosen.

3.7. Presentation of the objective function

The objective function is defined and can be used in an algorithm, in search for the optimal design with the following minimizing function:

$$\min F(\vec{D}) = \lambda_C M_C(\vec{D}) + \lambda_m M_m(\vec{D}) + \lambda_V M_V(\vec{D}) + p(\vec{D}) \tag{10}$$

Subject to:

$$
\begin{aligned}
& g_1(\vec{D}) \equiv 0.5 l_{battery} \le l_{system} \le 1.5 l_{battery} \\
& g_2(\vec{D}) \equiv 0.5 h_{battery} \le h_{system} \le 1.5 h_{battery} \\
& g_3(\vec{D}) \equiv 0.5 w_{battery} \le w_{system} \le 1.5 w_{battery} \\
& g_4(\vec{D}) \equiv \lambda_C + \lambda_m + \lambda_V = 1 \\
& g_5(\vec{D}) \equiv 0 + \lambda_C \le 1 \\
& g_6(\vec{D}) \equiv 0 \le \lambda_m \le 1 \\
& g_7(\vec{D}) \equiv 0 \le \lambda_V \le 1 \\
& h_1(\vec{D}) \equiv l_t h_t w_t = E(u\rho)_{fuel} \\
& h_2(\vec{D}) \equiv l_{fc} = w_{fc} = \sqrt{\frac{P_{nom}}{n_{fc} - V_{cell}} - \frac{1}{i_{cell}} - \frac{n_{fc}}{2}} \\
& j(\vec{D}) \equiv \theta = k\frac{1}{2}\pi, \text{ with } k \in R \\
& p(\vec{D}) = \begin{cases} 0 & \text{if } Obj_i \notin Obj_j \\ n_{intersection} & \text{other} \end{cases}
\end{aligned}
$$

where $g_1(D)$ to $g_3(D)$ define the search field in which the optimization may take place, and $g_4(D)$ to $g_7(D)$ define the field for the preference factors λ. The behavioral constraints $h_1(D)$ and $h_2(D)$ define the flexible components (explained in Sections 4.5 and 4.6). To decrease computation time the values for rotation of the objects is restricted to discrete values by $j(D)$. The penalty factor $p(D)$ is introduced to the function when objects from the component set intersect with each other.

3.8. Preference factors

To define the relative preference factor λ a conjoint analysis has been performed to give more insight in the factors influencing the user's choice when buying a cell-phone and a laptop computer [18]. The conjoint analysis is a method to find out the importance of several properties of a product. By applying the method it is possible to find out about the priorities of properties, as well as the referred value of each property itself [25]. Five properties are investigated and the average importance score for these properties are described in Table 1. We can use the average importance score as the preference factor for the five properties investigated.

In this research only three basic properties for optimization are defined namely volume, weight and costs. To define the preference for these basic properties the five properties investigated in the conjoint analysis are reduced to three. "Charge–time" and "time of use" is left out of the equation, and the resulting distribution is presented in the latter two columns of Table 1. The average importance score shows that for smaller products, like the cell phone, volume is the most important factor influencing the buying behavior of the consumer. For larger portable products, like the laptop computer this distinction is less visible.

3.9. Presentation of the optimization algorithm

Fig. 4 shows the flowchart of the algorithm which not only minimizes the objective function but also chooses the components based on simple performance specifications. The algorithm consists of three parts: the performance input and component selection, the multi-parametric optimization and the part presenting the results graphically and in data files.

3.10. Part 1: performance input and component selection

In part 1 the user has to input performance data of the application he/she wants to analyze. The performance data consists of a load-profile for one cycle and data of the benchmarked power source used in the device, like size, weight, costs and energy specifics. Based on these parameters the algorithm will calculate the required physical characteristics of all flexible components (as the fuel cells and fuel container) and design them, and make the choice for non-flexible components out of a database by matching the required performance with the actual characteristics of commercially available components (fuel and air pumps, and the intermediate accumulator). For every component the algorithm will choose one candidate, which fits with the performance needs of the component and has the lowest value of the objective function. All candidate components are listed in a *component set* which will be optimally placed in 3D space in part 2.

3.11. Part 2: multi parametric optimization

A combination of components is arbitrarily chosen and listed in a *component set*. For this set n initial solutions are defined. One solution is described in the form of a *Design vector D*, describing the placing of all components in space. The solutions are constrained by the design space defined by the different design constraints $g_i(D)$, $h_i(D)$ and $j_i(D)$. An initial design vector is defined $D[0,0]$, which is tested on possible intersection of objects (line–plane intersection). If the objects do not intersect a feasible solution is generated.

Table 1
Average importance score of the five properties derived from the conjoint analysis [18], and the used values for the algorithm (right two columns).

		Conjoint analysis		Numbers used in algorithm	
Type of product Example		Small handheld Cell phone	Large portable Laptop computer	Small handheld Cell phone	Large portable Laptop computer
λ_C	Costs	0.22	0.24	0.34	0.37
$\lambda_{t,charge}$	Charge time	0.17	0.18	–	–
$\lambda_{t,use}$	Time of use	0.18	0.17	–	–
λ_m	Weight	0.09	0.15	0.14	0.23
λ_V	Volume	0.34	0.25	0.52	0.40
$\Sigma\lambda$		1	1	1	1

The architecture of this feasible solution is analyzed by calculating the size of the bounding box, its volume, the costs of the system based on the components costs and the weight of the total system.

New design vectors $D[0,j]$ are generated, based on the initial design vector $D[0,0]$. The new design vectors are generated in the neighborhood of the initial design vector and are called *neighboring design vectors*, see Fig. 3. The design vector for five objects is defined as follows:

$$\vec{D}[i,j] = \left((\vec{r}_t[i,j], \vec{r}_r, \theta)_1, \ldots, (\vec{r}_r[i,j], \vec{r}_r\theta)_5\right) \tag{11}$$

where: r_t = a randomly generated vector for the translation of all objects depending on the dimensions of the benchmarked power source: $r_t = R(l_{datum}, w_{datum}, h_{datum})$, with $R \in [0,100]/100$; r_r = vector for the initial radius angles of all primary design vectors $D[i,0]$; θ = a randomly generated angle $\in [-\pi, -1/2\pi, 0, 1/2\pi]$; i = the primary design vector number, with $i = 1 \ldots n$; j = the neighboring design vector number, with $j = 1 \ldots m$

The following procedure is followed:

1. Components are selected based on the objective function (Part 1).
2. The rotation vector r_r and the angle to rotate about θ are fixed at start based on its intrinsic form.
3. The largest component is set as the base at start.
4. The primary design vector $D[0,0]$ is evaluated and a random cloud of neighboring design vectors $D[0,j]$ is generated within a maximum defined range r_0.
5. The fitness of every neighboring design vector is calculated by means of the objective function $F_j(D)$ plus a penalty function when intersection occurs $p(D)$.

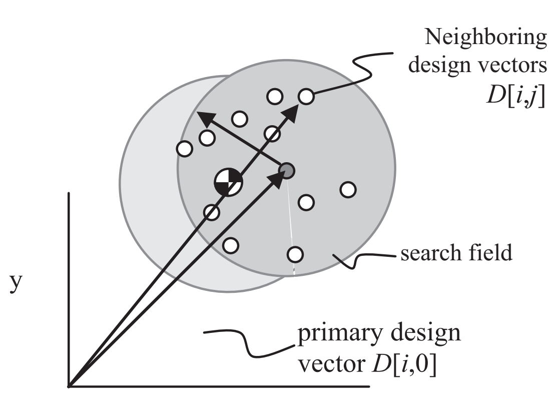

Fig. 3. A 2D representation of the primary design vector $D[i,0]$ for one object and the generated neighboring design vectors $D[i,j]$.

6. The "gravitational" mean of the cloud is calculated by:

$$\vec{r}_{cloud} = \left(\frac{\sum_{j=0}^{20} \vec{r}_{t_1} \cdot |\vec{F}_{ji}(D)|}{\sum_{j=20}^{20} |\vec{F}_{ji}(D)|}, \ldots, \frac{\sum_{j=0}^{20} \vec{r}_{t_{obj(t)}} \cdot |\vec{F}_{j_{obj(t)}}(D)|}{\sum_{j=0}^{20} |\vec{F}_{j_{obj(t)}}(D)|} \right)$$

   for $\text{obj}(t) = 1 \ldots 5$ objects

   where $j = 0$ is the fittest solution from the previous iteration and $j = 1 \ldots 20$ are the solutions belonging to the new generated cloud.
7. The cloud vector is subtracted from the primary translation vector r_t, consisting of all translation vectors of all objects, and the sign of every object in the design vector can be determined. A new primary design vector is generated with the new translation vector r_t equal to:

   $$\vec{r}_t[i+1, 0] = \vec{r}_t[i, 0] - sign(\vec{r}_t - \vec{r}_{cloud}) r_0$$

   With $r_0 = \alpha R$, where α is a randomly generated number in between 0 and 1, defining a limiting search field with a maximum radius R.
8. Repeat until the maximum number of generations is reached or convergence is reached.

3.12. Part 3: presentation of the results

Based on a single component set the optimal layout is defined by the final design vector $D[n,0]$. The architecture of this design is presented in a 3D graphic, together with all generations of best options made on the road towards this optimal (Fig. 4).

4. Case study: a DMFC power system for a MP3 player

To test the algorithm as described in the previous section a program is written to design an optimized DMFC system for a MP3 player. The program is written in Mathematica [26]. This section describes the algorithm by means of the case-study: the design of a DMFC power system powering the Samsung YP-Z5F MP3 player.

4.1. Performance input data

The data inputted by the user is in the form of load profile of one cycle. In the case of the MP3 player this is the coarsened load-profile of the WMA file (- - -) as pictured in Fig. 5. The power data is imported as a list of power in mW versus the time in seconds. The benchmarked battery specifications are inputted as a list of the capacity (mAh), the working voltage (V), the weight (g), price (€) and its dimensions (mm).

4.2. Introduction into component selection

With the data imported the algorithm will select non-flexible components from a database of commercially available components and designs flexible components matching the performance

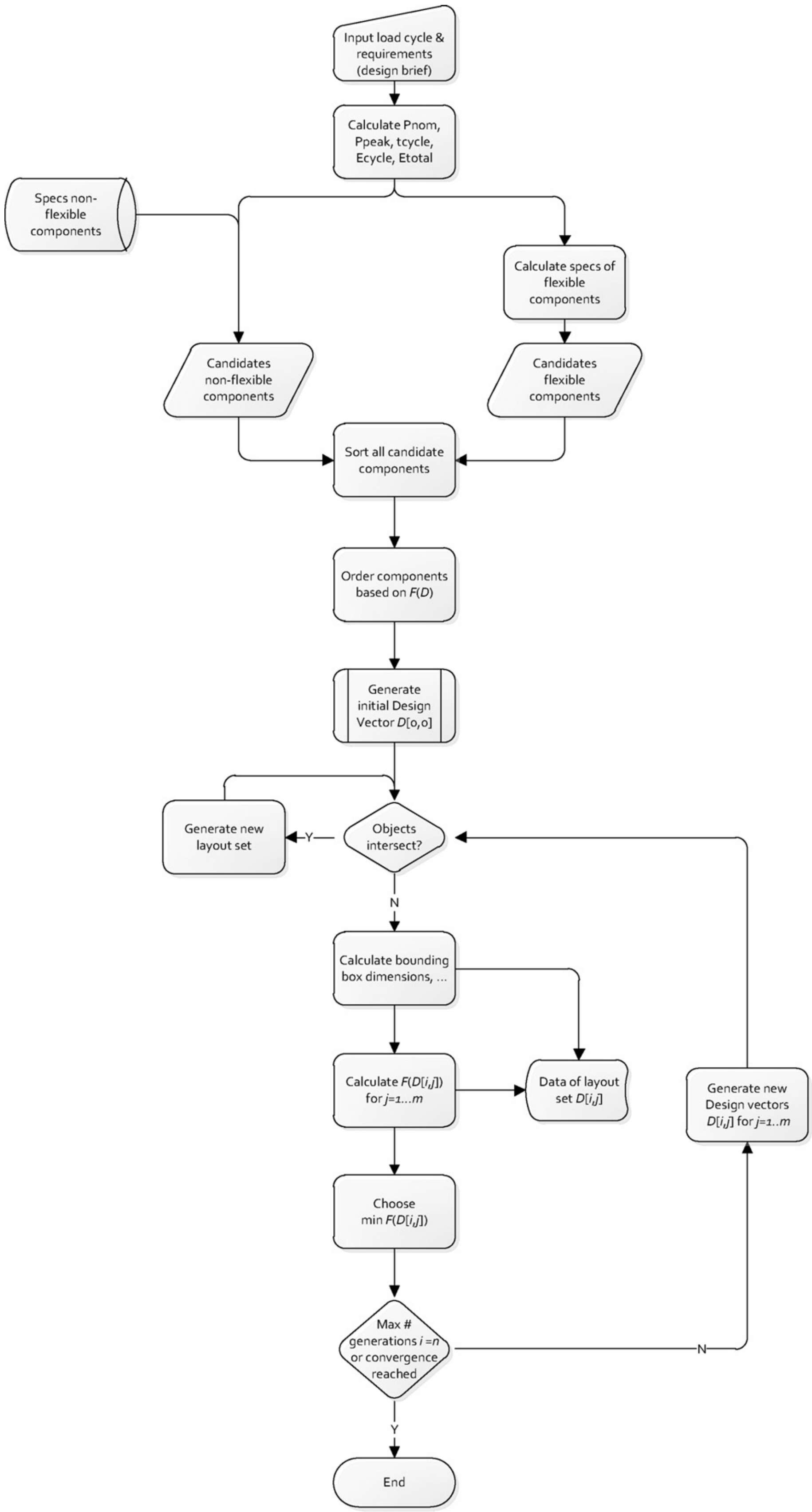

Fig. 4. Flowchart of the automated design procedure.

Table 2
An excerpt of the fuel-pump table in the component database.

Brand		Type	V (V)	P (mW)	Max flow (mL min^{-1})	l (mm)	w (mm)	h (mm)	m (g)	Price (€ 100+)
Bartels	MP5	Diaphragm, piezo	250	200	5	14	14	3.5	1	0.1
Bartels	MP6	Diaphragm, piezo	250	200	6	30	15	3.8	2	0.1
thinXXS	MDP1304	Diaphragm, piezo	5	250	10	25.4	26.2	7.5	3	0.1
thinXXS	MDP2205	Diaphragm, piezo	5	250	11.8	26.2	25.4	9	3	0.1
HNP	MZR2521	Annular gear, electromagnetic	18	3000	9	68.8	13	13	56	0.1
...	...	...	...	...	...	...	...	...	...	...

requirements of the device. In basis the DMFC system consists of five main components:

1. air pump (non-flexible)
2. fuel pump (non-flexible)
3. intermediate accumulator (non-flexible)
4. fuel cell stack or flat pack (flexible)
5. fuel tank (flexible)

Other components like the fuel-water mixer and mixing chamber, water condenser, air filters and other minor components are left out of this optimization because of lack of information about these components or the low impact on volume or weight. It is also assumed that the controller will be integrated on the PCB of the device.

Data from non-flexible components is extracted from a table (CSV file) imported in the code. A component is represented by its outer bound dimensions (length, width and height), its weight, its price, and performance specific variables. A component is represented as a parallelepiped (or a *Cuboid* in Mathematica) by only its height, width and length parameters. In Table 2 an excerpt for the fuel-pump table is shown. The choice for a specific component is based on its performance characteristics. For the air pump and the fuel pump this is the maximum flow (mL min^{-1}) and for the intermediate accumulator this is the voltage (V) and the capacity (mAh). The ordering is done on basis of the minimized value of these performance characteristics.

4.3. Air and fuel pump selection

The air and fuel pump are selected on their fuel-flow performance. For every pump in the table the maximum air or fuel flow is entered. On basis of the load profile, the air and fuel flow needed is calculated. Methanol crossover over the cell is hereby neglected.

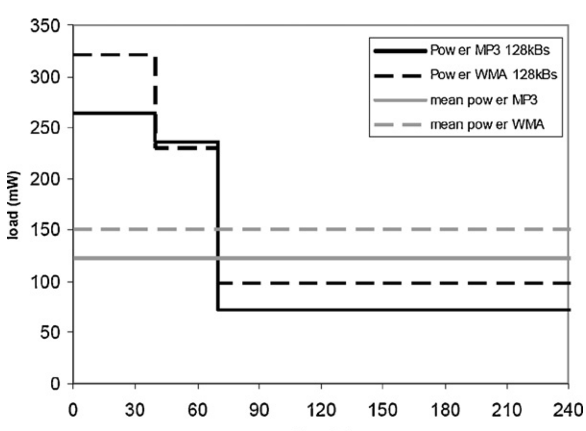

Fig. 5. Load profile for one WMA and MP3 file.

The following equations are used to calculate the mass (g min^{-1}) and volume flow (mL min^{-1}) [27,28]:

$$\dot{m} = xM\frac{P_{mean}}{V_{cell}n_eF}\lambda_{stoch}60 \tag{12}$$

And:

$$\dot{V} = \frac{\dot{m}}{\rho}$$

where: x = amount of moles used/produced in the reaction; P_{mean} = required mean power [mW]; V_{cell} = one cells voltage = 0.32 V; n_e = the amount of electrons per mole = 6; F = Faradays constant = 96485 Coulomb; ρ = density of the medium [g mL^{-1}]; M = molar mass [kg mole^{-1}]; λ_{stoch} = the stochiometric ratio at the anode and cathode.

In the reaction of the fuel cell three media will react, water (H_2O), methanol (CH_3OH) and oxygen (O_2), in our case as part of air. In Table 3 the values needed to calculate the fuel flows for these media are listed. Besides these values the mass and volume flows are calculated needed to match with the nominal power of the MP3 case (P_{nom} = 150 mW).

Besides for reaction water is also used as a carrier for the fuel to the membrane. Methanol is normally diluted in water at a percentage equal to 3%$_m$ (2.3%$_v$), resulting in an extra water flow needed:

$$\dot{V}_{H_2O|mix} = \frac{\dot{V}_{CH_3OH}}{2.3\%}$$

And thus the total fuel flow at the anode is equal to:

$$\dot{V}_{liquid} = \dot{V}_{CH_3OH} + \frac{\dot{V}_{CH_3OH}}{2.3\%} = 0.75\,\text{mL min}^{-1}$$

At the cathode the fuel flow consists of oxygen. Because the design does not include an oxygen tank but the oxygen from air is used, and thus air has to be pumped around. The oxygen percentage in air is equal to 21%, resulting in a fuel flow at the cathode equal to:

$$\dot{V}_{air} = \frac{\dot{V}_{O_2}}{21\%} = 14.6\,\text{mL min}^{-1}$$

Based on the calculated fuel flows at the anode and cathode the pumps can be selected, from a table consisting the dimensions, weight and, when available, price (for 100 items).

Table 3
Specific fuel characteristics for the used media in the DMFC.

	H_2O	CH_3OH	O_2
X	1	1	1.5
M kg mol^{-1}	0.018	0.032	0.032
λ	10	10	2
ρ g mL^{-1}	1.0	0.79	0.00143
$\dot{m}$ g min^{-1}	0.000146	0.01325	0.00398
$\dot{V}$ mL min^{-1}	0.000146	0.01677	2.7798

4.4. Intermediate accumulator selection

The intermediate accumulator is selected by matching the capacity of the battery with the required capacity when the battery has to be discharged and charged within one cycle, when the battery is discharged at a depth of discharge (DOD) equal to 80%:

$$C = \frac{1}{80\%\sum_{t=0}^{t_{cycle}} P - P_{nom}t|}$$

The dimensions, weight and, when available, price (for 100 items) is taken from the table.

4.5. Dimensioning the fuel cell

The fuel cell is the first flexible component in our component set. The fuel cells are designed as if they were custom build for the application. The designer has to indicate if the fuel cell is stacked or is designed with flat-pack architecture. The latter design is more voluminous but has the advantage of being thin, and thus fitting a thin product design.

The design of the fuel cell stack is based on the design from [29] working at a cell voltage of V_{cell} = 0.32 V at a current density of i_{cell} = 140 mA cm^{-2}. The number of cells needed is based on the maximum battery voltage:

$$n_{fc} = \left[\frac{V_{battery}}{V_{cell}}\right] \tag{14}$$

When assuming a flat pack design the required active area of the membrane can be calculated with:

$$A_{cell} = \frac{P_{nom}}{n_{fc} \cdot V_{cell}} \frac{1}{i_{cell}} \frac{n_{fc}}{2} \tag{15}$$

And thus the length and the width of all of the cells, when assuming a squared fuel cell flat pack architecture:

$$l_{cell} = w_{cell} = \sqrt{A_{cell}} \tag{16}$$

The thickness of the fuel cell flat pack is taken to be equal to the thickness of two endplates making use of the innovative monopolar architecture with a thickness of 0.8 mm for two cells [30].

Weight is calculated based on density numbers taken from the Motorola case [12] equal to ρ_{fc} = 2.078 kg L^{-1}. Prices are based on the price for one hundred square centimeters of Membrane Electrode Assembly (MEA) taken from [31] (May 2010), equaling \$356.36, and thus \$c3.56 or €c2.97 per mm^2. The MEA used in the design has an active area of 1420 mm^2, making the price for only this component equal to €42.17.

4.6. Dimensioning the fuel tank

The second flexible component is the fuel tank, which has to match with the energy need for a single charge. The dimensions of the fuel tank are flexible and can be used to fill up empty space. In our algorithm we have assumed the length and width of the tank be equal to the length and the width of the benchmarked power source. For the MP3 player this is equal to 66 and 33 mm. The thickness of the fuel tank is a result from the matching volume needed to store the required amount of energy (820 mAh at 3.7 V) and the amount of water described by c_{meoh} which is in our case equal to 1/2 (the amount of water equals the amount of methanol). The total thickness of the fuel tank is now equal to:

$$t_{tank} = \frac{E_{battery}}{c_{meoh}\rho_{E_{meoh}} l_{tank} w_{tank}}$$

The weight of the fuel tank can be calculated with the density of water (1 kg L^{-1}) and methanol (0.79 kg L^{-1}). Price is assumed to be equal to the price for a fill-pen refill, where a five-pack of 1.45 mL cartridges costs €1.90 [32], resulting in a price-density of: €c0.131 mm^{-3}.

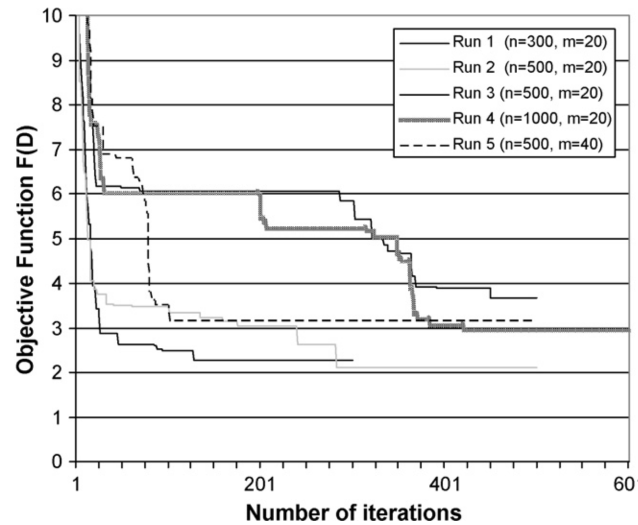

Fig. 6. Optimization of the objective function $F(D)$, for n primary design vectors $D[n,0]$ and m = 20–40 neighboring design vectors.

4.7. Ordering of components

A list of components is selected based on the performance requirements imported by the user. A list of compliant components is chosen and sorted on the minimum value of the objective function. For both the flexible components, the fuel cell and fuel tank designs match the performance requirements and thus no ordering is needed.

4.8. Test run results

The component selection is again based on the objective function and listed in Table 4. The algorithm is tested by conducting several runs, where the starting translation vector is changed. Three of five runs are plotted in Fig. 6, where all best values of $F(D)$ are plotted for every primary design vectors $D[i,0]$ with i = 0 . . . 300–500 and a cloud of n = 20 neighboring design vectors. Fig. 7 shows the design at start and finish of the Run 1 to 3. The 300–500 iteration runs take up 15–30 min on a Dell PC (Pentium Intel Core 2Duo CPU E8400@3Ghz, 1.97 GHz, 3.25GB RAM).

The algorithm is evaluated several times and the objective functions value is converging generally nearing 2 for run 1 and run 2. Run 3 converges to a higher value nearing 3. To test if this starting point will converge to the minimum value in new evaluations, this run is repeated. In Run 4 the number of evaluations n is increased from 500 to 1000 (Fig. 8a). In Run 5 the number of neighboring design vectors m is increased from 20 to 40 (Fig. 8b). The convergence of these test are also shown in Fig. 6, and do not see a convergence nearing 2.

4.9. Evaluation

The convergence of the algorithm is quick and minimizes to a low value of the objective function. The test is evaluated three times with different starting points. This test shows that the starting point influences the end-result, even after increasing the number of evaluations or the number of neighboring design vectors. Thus random generated start-points can converge to different local minima, which is not always the best case minimum. To test if the

Table 4
Overview of selected and designed components for the DMFC system applied in the Samsung YP5 MP3 player.

Component	Type	Length (mm)	Width (mm)	Height (mm)	Volume (mm^3)	Weight (g)	Price (EUR)
Air pump	Bartels MP5	14	14	3.5	689	0.80	n.a.
Fuel pump	ThinXXS MDP2205	26.2	25.4	9	5986	3.00	n.a.
Accumulator	Varta CR1/2AA	14.75	14.75	25.1	5460	11.50	n.a.
Fuel cell flat pack	Nafion 117 [29]	37.7	37.7	0.8	1141	2.37	42.17
Fuel tank	CH_3OH:H_2O = 1:1	66	33	2.53	5516	4.94	7.23
Total					18,793	22.60	>49.40

DMFC system is a good alternative to the benchmarked battery, the optimization run has to be repeated several times.

Viewing the end results in Figs. 7 and 8 show that the form of the fuel cell, which is the large squared form, is inefficiently chosen. If the fuel-cell has the form of a rectangular object, the packing ratio will decrease. The automated design procedure of this flexible object has to be redefined.

5. Discussion on the results

In the following sections the optimization algorithm, including the component selection, and the results from these optimizations are discussed based on volume, costs and weight.

5.1. Algorithm

In the case study presented in this paper multiple structural variants are generated for DMFC power systems powering the Samsung YP-Z5F MP3-player with a peak and nominal power of 360 and 120 mW, and a capacity of 3034 mWh. The structural variants are evaluated and optimized for the minimum value of $F(D)$. Three properties for optimization are introduced: volume, weight and costs, which are reduced to corresponding metrics M. To test the working of the algorithm the preference factor λ for volume is set to 1 and the rest (weight and costs) are set to 0.

The evolutionary algorithm proposed calculates the feasibility of a DMFC system with a low number of calculations converging to an improved objective function $F(D)$. The evolutionary algorithm also produces a design with a low value of the objective function to almost 2 whereas the theoretical minimum is 0.99 (see also Sec-

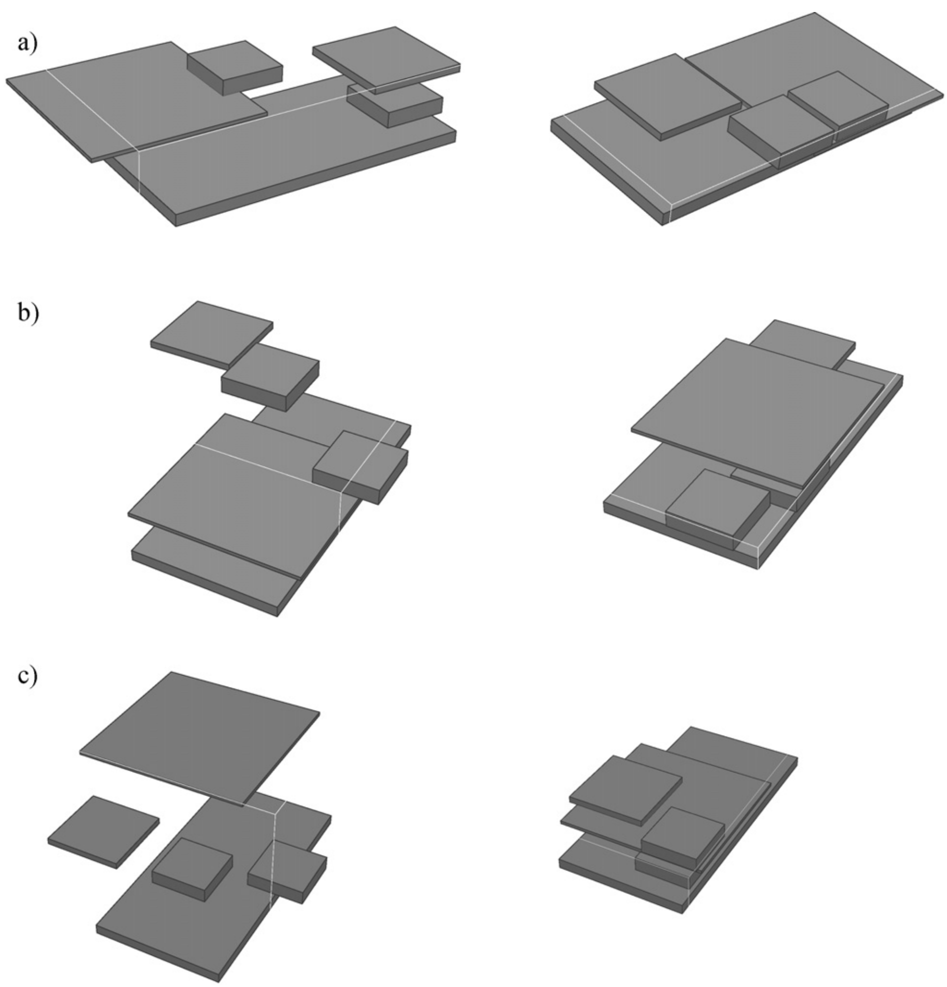

Fig. 7. Convergence of the algorithm for three algorithm evaluations with three different starting points (a, b and c), as shown at the left side. The results after the optimization are shown on the right side. (a) Run 1 where n = 300 evaluations and m = 20, starting with $F(D)$ = 13.51 and finishing at 2.28 (16 min). (b) Run 2 where n = 500 evaluations and m = 20, starting with $F(D)$ = 17.56 and finishing at 2.11 (27 min). (c) Run 3 where n = 500 evaluations and m = 20, starting with $F(D)$ = 25.61 and finishing at 3.68 (27 min).

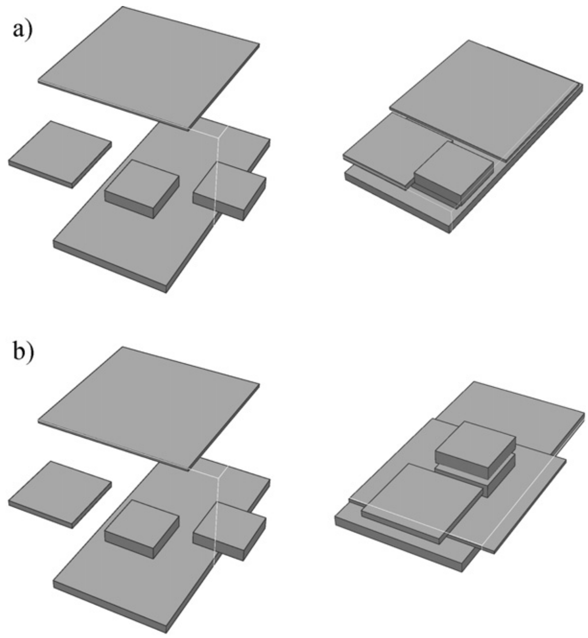

Fig. 8. Evaluation of Run 3 but with (a) an increase of the number of iterations, $n = 500 \rightarrow 1000$ (at $m = 20$) and an increased number of points in the cloud from $m = 20 \rightarrow 100$ ($n = 500$). (a) Run 3 again, where $n = 1000$ evaluations with $m = 20$, starting with $F(D) = 25.61$ and finishing at 2.84. (b) Run 3 again, where $n = 500$ evaluations with $m = 40$, starting with $F(D) = 25.61$ and finishing at 3.16.

tion 5.2). The algorithm starts with a randomly generated starting point, which not always results in the smallest value of the objective function. It is thus proposed to do several runs to test if the DMFC system is a good alternative to the benchmarked battery.

The algorithm is only useful when the load-curve is available. During the conceptual design process this is not always the case, and the designer should make a guess about the power over time for one cycle and over one charge. A small change in the load profile could mean a great difference in the selected component set, making the use of accurate load-curves a necessity when the designer wants to test the feasibility of a DMFC system. This makes the algorithm interesting for products already developed, where the load profile is known, and less for new to develop products, where the load-profile is based data from similar products or a previous version of the device.

5.2. Volume

The algorithm is used to optimize merely for volume. The results should present a final solution with a low amount of empty space, and a high packing ratio. The final design after the test run shows that this is not the case with a packing ratio nearing 2. The empty space in the generated DMFC system is more than 50% of the total volume. The sizing of the fuel-cell greatly influences this packing ratio. If the automated design of this flexible component takes the maximum width into account the packing ratio could decrease.

When comparing the total volume of only the components ($8659\,mm^3$) with the volume of the benchmarked battery ($8720\,mm^3$), it shows the selected component-set can lead to solution nearing that of the benchmark. If we look at the volume breakdown in Fig. 9 of all components we notice that the fuel tank takes up the most space. It must be noted that the tanks consists of a water and a methanol tank (50/50). If a 100% methanol tank is feasible than the value of this component will be halved. In the algorithm the interconnections like wiring and tubing is not taken into account, thus extra volume will be added.

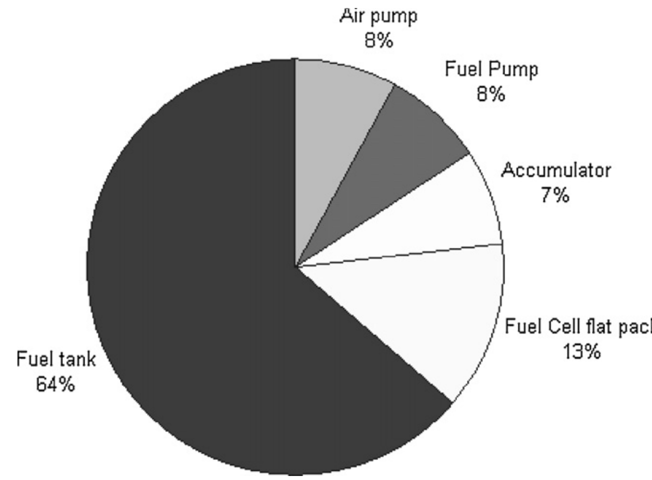

Fig. 9. Volume breakdown, without empty space, of the generated DMFC system ($E = 3034\,mWh$, $P_{syst} = 600\,mW$, $P_{fc} = 127\,mW$, $V_{total} = 18{,}428\,mm^3$, $V_{comp} = 8659\,mm^3$).

The DMFC system is only feasible with the chosen component set when empty space equals zero and no extra components or interconnections have to be added. An existing DMFC systems like the SFC Jenny [17] has an empty-space ratio of 15%. This product is optimized for volume and the amount of empty space is minimized to the maximum. Adding 15% to the current chosen component-set volume will result in a minimum feasible packing ratio of 1.15. Concluding from this the volume is a bottleneck in the current selected component-set, and thus will be a bottleneck for the feasibility of DMFC systems as an alternative for the lithium-ion battery when applied in the MP3 player case.

Note that costs and weight are not taken into account in the optimization algorithm, thus it is unknown if the selected components were selected as the primary component set when those factors were included. The algorithm is a good tool supporting the designer to place the components in the most opportune way, minimizing systems' bounding-box volume.

At the moment the algorithm makes use of only commercially available components. Besides the limited amount of alternatives, often candidates are over-dimensioned. The list should be updated and scalability of components should be an option added to the algorithm. When scalable components are introduced in the algorithm, it will produce designs which are feasible on the long term.

5.3. Weight

In Fig. 10 the weight break down is plotted for the DMFC system. The fuel tank is the heaviest component of the system. The total weight of the component-set selected is 10.7 g making this system half the weight of the benchmark (21 g), and thus in this respect very feasible. It must be taken into account that weight for wiring and plumbing is not yet added to the weight, which will result in a small increase of the total system weight.

5.4. Costs

In the last column of Table 4 the prices for all components are listed individually. The prices for non-flexible components are not always available, which makes it difficult to draw conclusions on the feasibility of the system compared to benchmarked battery. One thing can be noticed is the price for the fuel cell flat pack. The price is based on $100\,cm^2$ MEA [31] and is in this case a large contributor to the total price of the system. Compared to the price of the

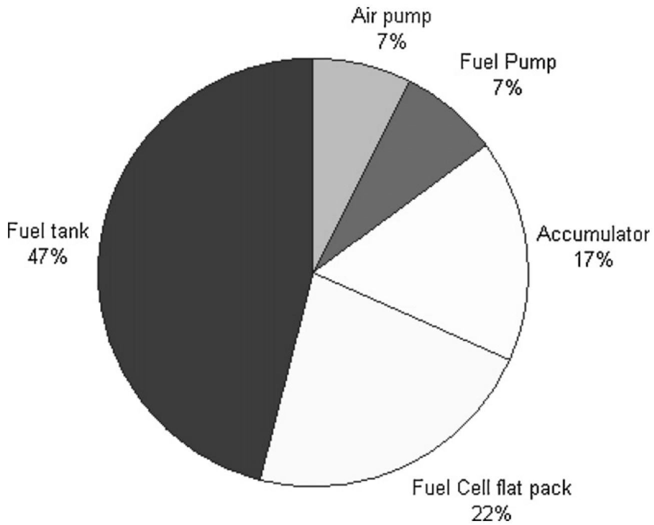

Fig. 10. Weight breakdown of the generated DMFC system (m_{total} = 10.71 g).

benchmarked battery, the price for only the MEA is almost 84% of the total price of the battery (€50).

According to Darnell [33] the MEA accounts for 40% of the total DMFC costs and 60% can be carried back to assembly and other components. Using this number the total price for the DMFC system would then be €105, making the initial price for the DMFC system a factor two higher than the lithium-ion battery used, at same specifications. This makes the DMFC system, at the moment, economically not competing with the benchmark.

Besides the high price for the MEA, prices for different components are not always available and liable for change. Because of the lack of price data for non-flexible components, the optimization with costs as part of the optimization function is not feasible within the algorithm at the moment. The component database should be extended with more optional components, and with more data, specifically on price.

6. Conclusions

In this paper an algorithm is proposed, and implemented in a Mathematica program, which consists of three parts: (1) selection of components into a component set, (2) evaluation of multiple structural variants and (3) presentation of the results.

In part 1 The best fitting component set is selected based on the objective function $F(D)$and used to generate multiple structural variants. The structural variants are optimized by minimizing the value of the objective function.

In part 2 several structural variants are produced, which are evaluated with the objective function. To test the program the optimization is only based on volume, and not on all three defined basic properties. An evolutionary algorithm is used to converge to a minimized value of the objective function in a low amount of calculations. The test run shows a convergence to a low value of the objective function nearing 2, in a low number of iterations. The convergence depends strongly on the starting point of the optimization, and thus several starting points have to be evaluated to be sure it will converge to the lowest value of several local minima.

In part 3 the design proposal is plotted in a 3D view. From these design proposals it can be concluded that the feasibility of the DMFC system strongly depends on the components' volume and costs. The total weight of the summed components, in de component-set, is 50% of the weight of the benchmarked battery, and thus no issue for the feasibility. The test run converges to the lowest value of the objective function nearing 2, whereas the theoretical minimum is 0.99. This means the DMFC system will be twice as large as the benchmarked battery. This can be decreased by a change the size of the fuel-cell from a squared to rectangular form, and make use of a 100% methanol fuel mix instead of a 50/50 water–methanol fuel tank.

The feasibility of price is difficult to test. For non-flexible components prices are not always available, and a small amount of different options are available. The prices for the components are based on commercially available sale prices when 100 pieces are bought. The price of the MEA is also based on sale prices from the fuelcellstore [31], and the MEA only will cost €42. This price for the MEA alone is 84% of the total price for the benchmarked battery. The total sale price of the component set selected by the algorithm is higher than €53. An estimate based on the figures given by Darnell [33] result in a total price for the DMFC system equaling €105. At same specifications this price is twice the price of the lithium-ion battery used, making the DMFC system not a commercially attractive alternative.

7. Recommendations

The amount of commercially available components which can be used in 0–100 W DMFC systems is low. Smaller components matching low-power DMFC systems have to be developed. To address this lack of components the algorithm could be introduced with scalable non-flexible components. These components are based on existing components but scaled up or down to match the required performance specifications. Scalable components give the designer an indication of the long-term feasibility and the constraints of having to develop new components.

The algorithm can evaluate multiple structural variants with the objective function as optimization variable. The use of tables and computerized producing structural variants is a clear way of making quick conceptual feasibility tests. In our case the feasibility of the DMFC system is tested as an alternative to the benchmarked rechargeable battery. The tables for non-flexible components are easy to update to current available components. The algorithm uses only the three basic properties for optimization, and extending the number of properties is proposed for the third-order model. Furthermore the algorithm evaluates only structural variants where components are represented by simple parallelepipeds. This representation does not follow the form of the actual component very accurate. To improve the accuracy of the model the objects should be represented by other forms like cylinders, but also by combination of forms. Interconnections are not taken into account in the second-order model and the third-order model should include these in the algorithm. A fourth order model can also include the influence of heat, fluid flow and other multi-physical parameters.

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