

# Impacts assessment and tradeoffs of fuel cell based auxiliary power units Part II. Environmental and health impacts, LCA, and multi-objective optimization

Francesco Baratto<sup>a,b</sup>, Urmila M. Diwekar<sup>a,\*</sup>, Davide Manca<sup>b</sup>

<sup>a</sup> *Departments of Bio, Chemical, and Industrial Engineering, Institute for Environmental Science and Policy, Center for Uncertain Systems: Tools for Optimization and Management, University of Illinois at Chicago, 851 S. Morgan St., Chicago, IL 60607, USA*

<sup>b</sup> *Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria Chimica “Giulio Natta”, Piazza Leonardo da Vinci 32, 20133 Milano, Italy*

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## Abstract

Auxiliary power units are devices that can provide all or part of the non-propulsion power for vehicles (space conditioning/heating, refrigeration, lighting, etc.). In the first part of this series of two papers on this topic, an integrated framework to identify and quantify trade-offs between cost effectiveness, efficiency, and environmental and health impacts of fuel cell power systems has been introduced. The present work concludes the description of the framework analyzing the components not discussed in part I: environmental impact assessment, health impact assessment, life cycle assessment (LCA), and multi-objective optimization. At the end of the paper the results obtained from the simulation of a base case design are presented and discussed.

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## 1. Introduction

In addition to high-profile applications such as automotive propulsion, the use of small fuel cell stacks (up to 5 kW) as auxiliary power units (APUs) for vehicles is receiving considerable attention. The main advantages of this kind of devices are to improve the power generation efficiency and to reduce emissions and noise when the vehicle is parked, and to extend the life of the main engine. They will probably supplant the common practice of idling trucks heavy-duty diesel engines. As stated earlier, although a lot of research is active in the fuel cell sector, the tradeoffs in terms of environmental and health impact as compared to the total cost and the system efficiency have never been systematically studied. An integrated framework that can automatically identify

and quantify these trade-offs has been developed and introduced in part I of this series of two papers [1]. The present work concludes the description of the framework analyzing the components not discussed in part I: environmental impact assessment, health impact assessment, life cycle assessment and multi-objective optimization (MOP). The last section of the paper is the analysis of the results obtained from the simulation of a base case design for the solid oxide fuel cell based auxiliary power units. Life cycle assessment and multi-objective optimization of the system will be subject of future publications.

## 2. Environmental impacts assessment

Environmental impact assessment can be defined as the process of predicting and evaluating the effects of an action or series of actions on the environment. The idea of including

\* Corresponding author. Tel.: +1 312 355 3277; fax: +1 312 996 5921.  
E-mail address: [urmila@uic.edu](mailto:urmila@uic.edu) (U.M. Diwekar).

environmental impact considerations into the evaluation of a process is widespread. However, not everyone may agree on the methodology by which one should calculate the environmental impacts of specific pollutants. What engineers need is an approximate relative ranking for the environmental impact of chemicals that can be used to make reasonable design or operation decisions. Cabezas et al. [2] developed a potential environmental impact (PEI) balance as a generalization of the WASTE REDUCTION (WAR) algorithm first introduced by Hilaly and Sikdar [3]. These authors introduced the concept of pollution balance, which quantifies the environmental impact of the pollutants in a process and, ultimately, serves as the basis for quantitative indicators that represent the environmental friendliness or unfriendliness of a given process. Converting the environmental friendliness or unfriendliness of a process into a quantitative measure makes WAR suitable for optimization problems. The potential environmental impact (PEI) of a given quantity of material is defined as the expected effect that this material would have on the environment if it were emitted into the environment. It should be noted that potential environmental impact is a conceptual quantity that cannot be directly measured. However, it can be estimated from measurable quantities [3–5], such as stream flow rates, stream compositions, and environmental impact parameters, such as toxicity.

The potential environmental impact balance for steady state processes after some modifications [5] is described by the expression

$$0 = \dot{I}_{\text{in}}^{(\text{cp})} - \dot{I}_{\text{out}}^{(\text{cp})} - \dot{I}_{\text{out}}^{(\text{ep})} + \dot{I}_{\text{gen}} \quad (1)$$

where  $\dot{I}_{\text{in}}^{(\text{cp})}$  and  $\dot{I}_{\text{out}}^{(\text{cp})}$  are the input and output rates of potential environmental impact to the chemical process,  $\dot{I}_{\text{out}}^{(\text{ep})}$  the output rate of PEI to the energy generation process, and  $\dot{I}_{\text{gen}}$  the rate of generation of potential environmental impact inside the process.  $\dot{I}_{\text{gen}}$  represents the creation or consumption of potential environmental impact by chemical reactions inside the chemical process.

In order to make explicit use of Eq. (1) in chemical process design, Mallick et al. [6] and Cabezas et al. [2] developed a first-order approximation to estimate the various terms in this expression from measurable quantities. The expressions are

$$\begin{aligned} \dot{I}_{\text{in}}^{(\text{cp})} &= \sum_i^{\text{EnvCat}} \alpha_i \dot{I}_i^{(\text{in})} \\ &= \sum_i^{\text{EnvCat}} \alpha_i \sum_j^{\text{Streams}} \dot{M}_j^{(\text{in})} \sum_k^{\text{Comps}} x_{kj} \psi_{ki}^s + \dots \end{aligned} \quad (2)$$

$$\begin{aligned} \dot{I}_{\text{out}}^{(\text{cp})} &= \sum_i^{\text{EnvCat}} \alpha_i \dot{I}_i^{(\text{out})} \\ &= \sum_i^{\text{EnvCat}} \alpha_i \sum_j^{\text{Streams}} \dot{M}_j^{(\text{out})} \sum_k^{\text{Comps}} x_{kj} \psi_{ki}^s + \dots \end{aligned} \quad (3)$$

where the sum over  $i$  is taken over all environmental impact categories, e.g., human toxicity, global warming, etc.,  $\alpha_i$  is the relative weighting of impact category  $i$  (used to combine PEI categories into a single PEI index),  $\dot{I}_i^{(\text{l})}$  is the potential environmental impact input ( $l = \text{in}$ ) or output ( $l = \text{out}$ ) associated with impact category  $i$ , the sum over  $j$  is taken over all streams into or out of the process,  $\dot{M}_j^{(\text{l})}$  is the mass flow rate of stream  $j$  into or out of the process, the sum over  $k$  is taken over chemical components,  $x_{kj}$  is the mass fraction of chemical  $k$  in stream  $j$ , and  $\psi_{ki}^s$  is the specific potential environmental impact of chemical  $k$  associated with environmental impact category  $i$ . The expression for  $\dot{I}_{\text{out}}^{(\text{ep})}$  is analogous to the expression for  $\dot{I}_{\text{out}}^{(\text{cp})}$ . The specific potential environmental impact of a chemical  $k$  associated with environmental impact category  $i$ ,  $\psi_{ki}^s$ , is estimated from measures of chemical environmental impact such as LD<sub>50</sub>, LC<sub>50</sub>, etc.

The WAR Algorithm uses several techniques for estimating the chemical environmental impact of a species. These estimations are used to describe relative potency of the chemicals in eight potential environmental impact categories. The impact categories used within the WAR algorithm are not inclusive of all possible impact categories, but do represent those categories that are considered to be the most significant environmental concerns to the chemical manufacturing industry. Impact categories that have not been incorporated into the WAR Algorithm include land use, resource depletion, noise, odor, etc.

The environmental impacts measures are based on the work of Young and Cabezas [5]. The measures of environmental impacts fall into four general categories: local human toxicity, local ecological toxicity, regional atmospheric, and global atmospheric. There are four local toxicological categories: human toxicity potential by ingestion (HTPI), human toxicity potential by inhalation or dermal exposure (HTPE), aquatic toxicity potential (ATP), terrestrial toxicity potential (TTP). There are two global atmospheric categories: global warming potential (GWP) and ozone depletion potential (ODP). There are two regional atmospheric categories: acidification or acid rain potential (AP) and photochemical oxidation or smog formation potential (PCOP).

We integrated WAR algorithm fully in Aspen so that it is no more necessary to go through the graphical interface of the EPA software [7] but the environmental impact is evaluated automatically after the flowsheet simulation.

### 3. Health impact assessment

The term “health risk” is defined by the qualitative and quantitative evaluation of health damage, disease or death resulting from the actual or potential presence and/or use of specific pollutants [8]. The main goal of risk analysis is to define the level of hazard posed to both individual human health and the health of whole population in the selected area.

The methodology used in this work strictly follows the procedure recommended by US EPA in Risk Assessment

Guidance for Superfund (RAGS) [9]. There are four steps in the baseline risk assessment process:

- data collection and analysis;
- exposure assessment;
- toxicity assessment;
- risk characterization.

The four steps will be briefly described in the following paragraphs. The entire procedure has been fully integrated in the framework and the health impact assessment is performed, after flowsheet convergence, by a separate Aspen “calculator block” developed for this purpose.

### 3.1. Data collection and analysis

Objective of the data collection and analysis is to gather specific site data that can be used to assess risks to human health. Each site, in fact, is unique and data collection strategies for one site may not be appropriate for another site [10]. Available site information must be reviewed to determine basic site characteristics, to identify potential exposure pathways and exposure points, and to help in the determination of data needs (including modeling needs). Land use categories that are applicable to most of the sites are: residential, commercial/industrial, and recreational. Because of the well-known pollution problem and the abundance of data, Los Angeles Air Basin (SoCAB) has been chosen as case study for simulations. The description of this case will be carried out in the follow up publication.

### 3.2. Exposure assessment

An exposure assessment is conducted to estimate the magnitude of actual and/or potential human exposures, the frequency and duration of these exposures, and the pathways by which humans are potentially exposed [9]. Conducting an exposure assessment involves different tasks: emission quantification, identification of exposed population and of all potential pathways of exposure, estimation of exposure point concentrations for specific pathways, and estimation of contaminant intakes of the exposed population for the specific pathways.

In the case taken into consideration, all the emission rates are computed through the simulation of the system in Aspen Plus. Adult and child populations in agricultural, industrial (only for adults) and residential scenarios were considered. Since the most relevant part of the emissions (which is the only one that was taken into account for the health impact assessment) is in the gaseous form, inhalation of outdoor air is the only combination pathway/media taken into consideration.

The exposure point concentration is the arithmetic average of the concentration that is contacted over the exposure period. It is regarded as a reasonable estimate of the concentration likely to be contacted over time. Exposure concentrations may be estimated by using monitoring data or predictive

chemical and transport models or a combination of the two approaches. The use of dispersion models is widespread in estimating exposure concentrations in air. EPA’s Guideline on Air Quality Models (“Guideline”) [11] addresses the regulatory application of air quality models for assessing criteria pollutants. ISC3 (Industrial Source Complex Model) [12] was chosen as dispersion model to convert emission rates into an estimate of the concentration likely to be contacted over time. This model was chosen due to several reasons:

- It is one of the preferred/recommended models by EPA.
- Its recommendations fit the case study (continuous toxic air emissions, 1 h to annual averaging times, transport distances less than 50 km, flat or rolling terrain, rural or urban areas).
- It is publicly available on the EPA’s Internet SCRAM website [13].
- Its source code is downloadable and written in FORTRAN language (the same required by the user module in Aspen).
- It allows different levels of complexity such as flat and complex terrain, possibility of chemical reactions, continuous and intermittent emissions, etc.

There are two basic types of inputs that are needed to run the ISC models. They are (1) the input runstream file, and (2) the meteorological data file. Since the ISC models are especially designed to support the EPA’s regulatory modeling programs, the regulatory modeling options, as specified in the Guideline on Air Quality Models, are the default mode of operation for the models. No buildings information was input and no chemical decomposition or decay of any species was considered. Urban environment was modeled using the complex terrain algorithm. The exhaust tailpipe of a class 8 truck was estimated as 4 m height with a diameter of 20 cm. The meteorological data file refers to Los Angeles, CA in 1989 and is retrieved from ref. [14].

Intakes are expressed as the amount of chemical at the exchange boundary (e.g., skin, lungs, gut) and available for absorption. The general expression for calculating intakes is:

$$I = C \frac{C_R E_F E_T E_D}{A_T B_W} \quad (4)$$

where  $I$  is intake ( $\text{mg kg}^{-1}$  body weight  $\text{day}^{-1}$ ),  $C$  the average concentration contacted over the exposure period (e.g.,  $\text{g m}^{-3}$ ),  $C_R$  the contact rate: the amount of contaminated medium contacted per unit time (e.g.,  $\text{m}^3 \text{h}^{-1}$ ),  $E_F$  the exposure frequency (e.g.,  $\text{days year}^{-1}$ ),  $E_T$  the exposure time (e.g.,  $\text{h day}^{-1}$ ),  $E_D$  the exposure duration (e.g., year),  $B_W$  the body weight (kg), and  $A_T$  is the averaging time (days).

All the parameters were retrieved from ref. [15]. Concerning the average concentration contacted ( $C$ ) during a long-term time, the one-hour maximum concentration is not usually a reasonable estimate [9]. To get an estimate of the long-term (annual) concentration from the value of the short-term concentration, the procedure described in [16,17] for screening techniques was followed. This, applied to the considered

case, leads to the following formula:

$$C_{\text{Annual}} = C_{1\text{h}} \times 0.8 \times \frac{6 \text{ h/day} \times 303 \text{ days/year}}{8760 \text{ h/year}} \quad (5)$$

### 3.3. Toxicity assessment

The purpose of the toxicity assessment is to provide, where possible, an estimate of the relationship between the extent of exposure to a contaminant and increased likelihood and/or severity of adverse effects. The adverse effect can be classified in chronic, acute and carcinogenic. A reference dose ( $R_fD$ ) is the toxicity value used most often in evaluating non-carcinogenic-chronic effects. A chronic  $R_fD$  is defined as an estimate (with uncertainty spanning of an order of magnitude or greater) of a daily exposure level for the human population, including sensitive subpopulations, that is likely to be without an appreciable risk of deleterious effects during a lifetime [9].  $R_fDs$  differ according to the exposure route. A slope factor (SF) is the toxicity value most often used to evaluate potential human carcinogenic effects. An SF is a plausible upper-bound estimate of the probability of a response per unit intake of a chemical over a lifetime. The slope factor is used to estimate an upper-bound probability of an individual developing cancer as a result of a lifetime of exposure to a particular level of a potential carcinogen [9]. The slope factor is usually, but not always, the upper 95th percent confidence limit of the slope of the dose–response curve and is expressed as  $(\text{mg kg}^{-1} \text{ day}^{-1})^{-1}$ . SFs differ according to the exposure route. An acute reference exposure level (REL) is the toxicity value used most often to evaluate acute effects. California Environmental Protection Agency (CalEPA) defines the REL as a concentration level at (or below) which no health effects are anticipated [18], a concept that is substantially similar to EPA's non-carcinogenic effect for single event exposure. All the  $R_fDs$  and SFs are taken from the online database risk assessment information system (RAIS) [19], which contains information taken from EPA's integrated risk information system (IRIS) [20], the health effects assessment summary tables (HEAST) [21], EPA peer reviewed toxicity values (PRTVs) database, and other information sources in the hierarchy given by EPA. Other sources were consulted only for the species considered in the simulation not included in RAIS. All the REL values are taken from [22]. Table 1 shows the toxicity values with reference and assumptions for the species considered in the simulations. The cells without any specified value refer to data not found in any database. For such data, a value of 0 was assumed.  $R_fD$  or REL equal to 0 stands for no hazard and not infinite hazard index or quotient, as it should be mathematically (Table 1).

### 3.4. Risk characterization

In this final step, the toxicity and exposure assessments are summarized and integrated into quantitative and qualitative expressions of risk [9]. For carcinogens, risks are estimated

as the incremental probability of an individual developing cancer over a lifetime as a result of exposure to the potential carcinogen (i.e., incremental or excess individual lifetime cancer risk). The linear low-dose equation is:

$$\text{risk} = I \times \text{SF} \quad (6)$$

where risk is a unitless probability of an individual developing cancer,  $I$  the daily intake averaged over 70 years, and SF is slope factor.

However, this linear equation is valid only at low risk levels (i.e., below estimated risks of 0.01). For sites where chemical intakes might be high (i.e., risk above 0.01), an alternate calculation equation should be used [24]:

$$\text{risk} = 1 - \exp(-I \times \text{SF}) \quad (7)$$

The measure used to describe the potential for non-carcinogenic toxicity to occur in an individual is not expressed as the probability of an individual suffering an adverse effect. The potential for non-carcinogenic effects is evaluated, instead, by comparing an exposure level over a specified time period (e.g., life time) with a reference dose derived for a similar exposure period. This ratio of exposure to toxicity is called hazard quotient:

$$\text{hazard quotient} = \frac{I}{R_fD} \quad (8)$$

where  $I$  is daily intake and  $R_fD$  is reference dose.

The non-cancer hazard quotient assumes that there is a level of exposure (i.e.,  $R_fD$ ) below which it is unlikely for even sensitive populations to experience adverse health effects. If the exposure ( $I$ ) exceeds this threshold (i.e., if  $I/R_fD$  term exceeds unity), there may be concern for non-cancer effects. As a rule, the greater the value of  $I/R_fD$  above unity, the higher the level of concern.

For acute responses the concept of hazard index is introduced. The hazard index is analogous to the hazard quotient for chronic effects, but in this case the concentration of the species (and not the intake) is compared to the reference exposure level:

$$\text{hazard index} = \frac{C}{\text{REL}} \quad (9)$$

where  $C$  is species concentration and REL is reference exposure level.

At most of the sites, one must assess potential health effects of more than one chemical (both carcinogens and other toxicants) at the same time. Since information on specific mixture is rarely available, the total risk is obtained adding the values of the single risks, hazard quotients or hazard indexes respectively [25]. This method, of course, shows several limitations that must be acknowledged. For example, it sums terms derived from data with different toxicological significance or referring to different compounds that are not expected to induce the same type of effect.

Table 1  
Toxicity values for the components considered in the simulations

Component name	REL acute response ( $\mu\text{g m}^{-3}$ )	Inhalation R <sub>f</sub> D ( $\text{mg kg}^{-1} \text{day}^{-1}$ )	Inhalation SF ( $\text{kg day mg}^{-1}$ )	Notes
Nitrogen		0 <sup>a</sup>	0 <sup>a</sup>	
Oxygen		0 <sup>a</sup>	0 <sup>a</sup>	
Water		0 <sup>a</sup>	0 <sup>a</sup>	
Sulfur				
Hydrogen		0 <sup>a</sup>	0 <sup>a</sup>	
Carbon-monoxide	23000 <sup>b</sup>			
Carbon-dioxide		0 <sup>a</sup>	0 <sup>a</sup>	
Methane		0 <sup>a</sup>	0 <sup>a</sup>	
N-Nonane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Decane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Undecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Dodecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Tridecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Tetradecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Pentadecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Hexadecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Heptadecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Octadecane		0.286 <sup>c</sup>	0 <sup>c</sup>	(1)
N-Nonadecane		0 <sup>c</sup>	0 <sup>c</sup>	(2)
N-Eicosane		0 <sup>c</sup>	0 <sup>c</sup>	(2)
Ethane		0 <sup>a</sup>	0 <sup>a</sup>	
Propane		0 <sup>a</sup>	0 <sup>a</sup>	
N-Butane	23700000 <sup>a</sup>			
N-Pentylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(3)
N-Hexylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(3)
N-Heptylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(3)
N-Octylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(3)
N-Nonylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(3)
N-Decylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(3)
N-Undecylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(4)
N-Dodecylbenzene		0.114 <sup>c</sup>	0 <sup>c</sup>	(4)
Naphthalene		0.000857 <sup>c</sup>	0 <sup>c</sup>	
1-Methylnaphthalene		0.000857 <sup>c</sup>	0 <sup>c</sup>	(5)
1-Ethyl-naphthalene		0.114 <sup>c</sup>	0 <sup>c</sup>	(4)
1-N-Propylnaphthalene		0.114 <sup>c</sup>	0 <sup>c</sup>	(4)
1-N-Butylnaphthalene		0.114 <sup>c</sup>	0 <sup>c</sup>	(4)
Hydrogen-sulfide	42 <sup>b</sup>	0.000571 <sup>c</sup>	0 <sup>c</sup>	
Benzene	1300 <sup>b</sup>	0.00857 <sup>c</sup>	0.0273 <sup>d</sup>	
1,3-Butadiene		0.000571 <sup>c</sup>	0.105 <sup>d</sup>	
Nitrogen-dioxide	470 <sup>b</sup>	0 <sup>c</sup>	0 <sup>c</sup>	
Nitric-oxide	470 <sup>b</sup>	0 <sup>c</sup>	0 <sup>c</sup>	(6)
Ammonia	3200 <sup>b</sup>	0.0286 <sup>d</sup>	0 <sup>c</sup>	
Formaldehyde	94 <sup>b</sup>	0 <sup>c</sup>	0.0455 <sup>d</sup>	
Isobutane		0 <sup>a</sup>	0 <sup>a</sup>	
N-Pentane		0.0571 <sup>c</sup>	0 <sup>c</sup>	(7)
N-Hexane		0.0571 <sup>c</sup>	0 <sup>c</sup>	
N-Heptane		0.0571 <sup>c</sup>	0 <sup>c</sup>	(7)
N-Octane		0.0571 <sup>c</sup>	0 <sup>c</sup>	(7)
Carbon-graphite	65 <sup>b</sup>		3850 <sup>b</sup>	(8)
Sulfur-dioxide	660 <sup>b</sup>			
Sulfur-trioxide	120 <sup>b</sup>			
Nitrous-oxide				

Notes: (1) Considered as “Total Petroleum Hydrocarbons” (aliphatic with medium molecular weight); (2) considered as “Total Petroleum Hydrocarbons” (aliphatic with high molecular weight); (3) considered as “Total Petroleum Hydrocarbons” (aromatic with medium molecular weight); (4) assumed as “Total Petroleum Hydrocarbons” (aromatic with medium molecular weight); (5) assumed equal to naphthalene; (6) REL assumed equal to NO<sub>2</sub>; (7) considered as “Total Petroleum Hydrocarbons” (aliphatic with low molecular weight); (8) assumed as particulate from diesel engine. REL from NAAQS [23] for PM<sub>2.5</sub> 24 h.

<sup>a</sup> Canadian Center for occupational Health and Safety, CHEMINFO, Chemical Profiles created by CCOHS, <http://www.ccinforweb.ccohs.ca/chempendum/search.html>.

<sup>b</sup> California Environmental Protection Agency, Air Resources Board, Stationary Source Division: Health Risk Assessment Program database. March 1996.

<sup>c</sup> Risk Assessment Information Service, RAIS, <http://www.risk.lsd.ornl.gov/homepage/>.

<sup>d</sup> USEPA, National Center for Environmental Assessment: Integrated Risk Information System (IRIS), Cincinnati, OH.

#### 4. Life cycle assessment

Life cycle assessment (LCA) is a systematic tool to provide information on the environmental impacts of alternative materials, products, processes and services. LCA attempts to trace out the major stages and processes involved over the entire life cycle of a product in a “cradle-to-grave” approach. “Cradle-to-grave” begins with the gathering of raw materials from the earth to create the product and ends at the point when all materials are returned to the earth. LCA evaluates all stages of a product’s life from the perspective that they are interdependent, meaning that one operation leads to the next. It enables the estimation of the cumulative environmental impacts often including impacts not considered in more traditional analyses (e.g. raw material extraction, material transportation, ultimate product disposal, etc.). By including the impacts throughout the product life cycle, LCA provides a comprehensive view of the environmental aspects of the product or process and a more accurate picture of the true environmental trade-offs in product selection [26].

The term “life cycle” refers to the major activities in the course of the product’s life-span from its manufacture, use, maintenance, and final disposal; this includes the raw material acquisition required to manufacture the product. The LCA process is systematic and phased approach. It consists of four components: goal definition and scoping; inventory analysis; impact assessment; interpretation [26]. Performing an LCA can be resource and time intensive. Gathering the data in particular can be problematic, and the availability of data can greatly impact the accuracy of the final results. Therefore, it is important to weigh the availability of data and the time necessary to conduct the study against the projected benefits of the study. LCA will not determine which product or process is the most cost effective or works the best. Therefore, the information developed in an LCA study should be used as one component of a more comprehensive decision process assessing the trade-offs with cost and performance.

The life cycle of an SOFC based APU is defined to include all the steps required to provide the fuel, to manufacture the device, and to operate and maintain the vehicle throughout its lifetime up to disposal and recycling. The life cycle stages of an SOFC based APU system can be grouped in four components: system production, fuel life cycle, system operation and dismissing. Different models have been used for the different stages of the life cycle. This component of the framework and the results that have been obtained will be deeply discussed in a follow up publication.

#### 5. Multi-objective optimization

As presented so far, there are several goals or objectives that need to be achieved for designing and operating fuel cell based APUs. The system should have as high efficiency as possible, but also be economically viable with cost or profits competitive with the existing technology. Not only should

the environmental impacts of the chemicals released during the process be as low as possible, but also the human health impact has to be minimum. Moreover, as it is explained in Section 3, the health impact consists of three components (carcinogenic, chronic and acute effects) which are completely independent objectives. Other factors like LCA considerations (Section 4) might also be taken into consideration. This becomes an extremely challenging multi-objective problem (MOP) and its solution leads to the quantification of the trade-offs between the different objectives. The fact that these multiple objectives are often conflicting in nature and can have completely different trends with respect to multiple process variables makes the representation and analysis of the trade-off information an extremely formidable task.

An MOP is any decision problem that involves a set of objectives instead of a single one. There is a large array of analytical techniques for solution of multi-objective optimization problems. MOP methods are generally divided into two basic types: preference-based methods and generating methods [27]. Preference-based methods (like goal programming) attempt to quantify the decision-maker’s preference, and with this information, the solution that best satisfies the decision-maker’s preference is identified. Generating methods, such as the weighting method and the constraint method, have been developed to find a set of preferred solutions or the trade-off surface, also known as the Pareto set. For each of these solutions, it is impossible to improve one objective without sacrificing the value of another one. Many of the preference based methods suffer from an information inadequacy: they require the decision-maker to state preferences before he or she knows what the choices are. The more desirable scenario would be to present the decision-maker with the set of Pareto optimal solutions determined independent of a priori or interactive preferences. That is the main reason of the choice to focus on generating methods and in particular on constraint method. This method offers the advantages of better control over exploration of the Pareto set and of being able to locate points anywhere along the Pareto surface. The disadvantage is that the computational cost increases rapidly with the number of objectives. A new multi-objective nonlinear programming algorithm called minimizing number of single objective optimization problems (MINSOOP) [28], that is based on the traditional constraint method but can obtain significant computational savings, has been used to overcome this problem. The basic strategy of constraint method is to transform the multi-objective optimization problem into a series of single objective optimization problems. The idea is to pick one of the objectives to minimize while each of the others is turned into an inequality constraint with parametric right-hand sides. Solving repeatedly for different values of the parametric right-hand sides leads to the Pareto set.

There are usually many (infinite in number) Pareto optimal solutions. Therefore, instead of finding the complete Pareto set, in practice it is often sufficient to find a true representation of it through an approximate discrete set of Pareto-optimal points. Recently Kalagnanam and Diwekar [29] de-

veloped an efficient sampling technique called the Hammersley sequence sampling (HSS) technique based on a quasi-random number generator. It uses the Hammersley points to uniformly sample a  $(k-1)$ -dimensional hypercube, and the results revealed that the Hammersley points provide the optimal location for the sample points so as to obtain better uniformity in the  $(k-1)$ -dimension. Moreover, it preserves the property of Monte Carlo method where the number of samples required to obtain given accuracy of estimates does not scale exponentially with number of variables. MINSOOP algorithm uses the Hammersley sequence sampling to generate combinations of the right-hand-side for the adjunct constraints.

In order for the optimization to be effective and meaningful, the decision variables that are varied are those that have significant effect on the objectives. A sensitivity study needs to be carried out in order to quantify the effect of each input parameter on the objectives. Usually, partial derivatives represent the sensitivity analysis. However, for highly non-linear problems like the one we are dealing with, this only provides local sensitivity. In order to circumvent this problem, a sampling approach based on partial rank correlation coefficients (PRCC) is used. The partial correlation coefficients calculated on ranks are a good measure of the strength of monotonic relations between inputs and outputs, whether linear or not [30], and provide sensitivity for the whole range unlike partial derivatives normally used in this analysis. Input variables with higher PRCC have stronger input relationship.

## 6. Analysis of the base case

This section shows in detail the results obtained from the simulation of a base case design of an SOFC based APU. This base case will be improved through optimization and this is subject of follow up publications. Life cycle considerations are not included in this analysis.

The input parameters for this base case have been already presented in part I [1]. The two input streams of each APU, diesel, and air intakes, have a volumetric flow of  $1.444361 \text{ h}^{-1}$  and  $73.55801 \text{ m}^3 \text{ h}^{-1}$  (temperature  $25^\circ\text{C}$  and pressure 1 bar), respectively.

Table 2 shows the component flows from the two outlet streams: the exhaust gases and the excess water. As it can be seen the amount of excess water is negligible and  $\text{CO}_2$  is the major pollutant emitted.

Table 3 presents the overall performance results per cell. The output of the cell is greater than 5 kW because the cell has to power the air compressor and the pumps (parasitic loads). The fuel cell efficiency is defined as the power output divided by the lower heating value (LHV) of the fuel entering the cell. The reformer efficiency is defined as the ratio between the LHV of the species of interest leaving the reactor (hydrogen, methane, ethane and carbon monoxide) and the LHV of the mixture entering the reactor.

Table 2  
Components flow from outlet streams

Component	Exhaust gases ( $\text{mg s}^{-1}$ )	Excess water ( $\text{mg s}^{-1}$ )
$\text{N}_2$	6.758722	$3.18\text{E}-15$
$\text{O}_2$	1.663157	$1.94\text{E}-14$
$\text{H}_2\text{O}$	0.199467	$8.88\text{E}-08$
CO	0.000441	0
$\text{CO}_2$	0.363437	$1.94\text{E}-14$
$\text{CH}_4$	$2.78\text{E}-10$	0
$\text{NO}_2$	0.000123	$3.99\text{E}-14$
$\text{NH}_3$	$5.28\text{E}-06$	$1.74\text{E}-14$
$\text{CH}_2\text{O}$	$4.18\text{E}-08$	0
Total	8.985354	$8.88\text{E}-08$

Table 3  
Efficiencies and fuel cell performances of the base case

Overall efficiency (%)	37.4
Fuel cell efficiency (%)	47.4
Reformer efficiency (%)	90.5
Cell power output (W)	5734
Voltage (V)	0.687
Current density ( $\text{A m}^{-2}$ )	6103.8
Cell area ( $\text{m}^2$ )	1.3678

Various cost values are presented in Table 4. These cost values reflect the cost of a single APU. As it can be seen, fuel consumption over 5 years (9090 h) is the most relevant part. Therefore in this design the operating cost is the most important share of the total cost (61%), while the initial investment (manufacturing cost + installation) is only about US\$ 4600 (33%).

Health and environmental impacts are recorded in Tables 5 and 6, respectively. The simulations refer to the South California Air Basin case study. The details about this case study will be object of future publications. Briefly, 2700 APUs are assumed to be working at the same time and the source points are 27 truck rest areas of the region. Concentra-

Table 4  
Cost results for one APU in the base case design

Item	Cost (US\$)
SOFC stack	586.8
Reformer	125.8
Tail gas burner	37.4
Air compressor	250.7
Fuel pump	109.0
Recirculation pump	109.0
Air pre-heater	269.9
Steam generator	20.1
Exhaust condenser	265.2
Balance of system	450.0
Indirect cost	191.2
Contingencies	667.1
Manufacturing	3082.2
Installation	1500.0
Maintenance	454.0
Desulfurizer repl.	350.0
Diesel (5 years)	8532.3
Total cost	13918.5

Table 5  
Health impact assessment for the base case

	Population	Impact	Scenario in which maximum risk is detected
Cancer risk	Adult	6.6498E–12	Residential
	Child	3.7254E–12	Residential
Chronic hazard quotient	Adult	1.3269E–05	Industrial
	Child	3.8075E–06	Residential
Acute hazard index		1.1631E–04	Residential

tions are computed over a uniform grid with 15 km spacing and actual terrain and meteorological data are used for more reliable results.

Some values for the generation rate of potential environmental impact are negative. This means that the species that are emitted are less harmful in that particular category than diesel components (input). The greater contribution to the total output PEI comes from the Aquatic Toxicity Potential, primarily due to the emissions of carbon dioxide and NO<sub>x</sub>.

Chronic hazard quotients and acute hazard indexes are far below unity and cancer risk is far below 10<sup>–6</sup> (considered the safety limit [31]). This fact means that no level of danger is

Table 6  
Rates of PEI for the base case

Input rate of PEI	PEI/s
Human toxicity potential by ingestion	0.096994
Human toxicity potential by inhalation or dermal exposure	0.000152
Ozone depletion potential	0.000000
Global warming potential	0.000000
Photochemical oxidation potential	0.132938
Acidification potential	0.000000
Aquatic toxicity potential	1.720817
Terrestrial toxicity potential	0.096994
Total input rate of PEI	2.047894
Output rate of PEI	PEI/s
Human toxicity potential by ingestion	0.000039
Human toxicity potential by inhalation or dermal exposure	0.000134
Ozone depletion potential	0.000000
Global warming potential	0.000841
Photochemical oxidation potential	0.000000
Acidification potential	0.000684
Aquatic toxicity potential	0.099873
Terrestrial toxicity potential	0.000039
Total output rate of PEI	0.101610
Generation rate of PEI	PEI/s
Human toxicity potential by ingestion	–0.096955
Human toxicity potential by inhalation or dermal exposure	–0.000018
Ozone depletion potential	0.000000
Global warming potential	0.000841
Photochemical oxidation potential	–0.132937
Acidification potential	0.000684
Aquatic toxicity potential	–1.620944
Terrestrial toxicity potential	–0.096955
Total input rate of PEI	–1.946284

posed by SOFC based APUs in the receptor points in which concentrations were computed. Health effects are a consequence of the emission of NO<sub>x</sub>, ammonia, carbon monoxide and formaldehyde (which is the only emitted species with carcinogenic effect).

## 7. Conclusions

This paper concludes the description of the main components of the integrated framework that has been developed in order to identify and quantify trade-offs between cost effectiveness, efficiency and environmental and health impacts of fuel cell power systems. The components described in this paper are useful to quantify the environmental impact, the health impact and to perform a life cycle analysis. Finally the last component of the framework, multi-objective optimization, is the one which is helpful to find the trade-offs between the different objectives that need to be achieved simultaneously: minimum cost, maximum efficiency, and minimum health and environmental impacts. The environmental impact is quantified using the WAR algorithm [2] developed by EPA and integrated in the framework. The health impact, instead, is computed strictly following the EPA recommendations contained in RAGS [9]. With the help of a dispersion modeler, concentrations of different pollutants are calculated over a grid of receptor. This information, together with the data from a toxicity database, is used to compute chronic and acute effects and carcinogenic risk for a population of adults and children in different scenarios. The process has been completely integrated into the framework.

At the end of the paper the integrated framework is applied to a base case design of the SOFC based APU. The results show that the main pollutant emitted is carbon dioxide and the health risks for all the effects are far below the safety limits.

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