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Development of the MATLAB Tool for Optimization of the Nuclear Hybrid Energy System Dedicated for Hydrogen Production

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ABSTRACT

The paper presents the development process, features, and example application of the tool for optimization of the Hybrid Energy System (HES) with nuclear reactors dedicated to hydrogen production. The tool was developed in the MATLAB environment with Optimization Toolbox^{TM} and Global Optimization Toolbox^{TM}. At the current stage of development, it solves Linear Programming and Mixed Integer Linear Programming problems with a single objective using a standard solver or multi-objective with genetic algorithms. It applies optimization algorithms to obtain a HES configuration fulfilling predefined objectives and constraints.

The work was focused on large-scale systems with nuclear reactors coupled with various hydrogen production technologies. The internal database of possible technologies and their performance was created based on available literature. The work considers HES systems that utilize different nuclear reactor technologies like Gen-III and Gen-IV reactors and different hydrogen production technologies, including Low-Temperature Electrolysis (LTE) and High-Temperature Electrolysis (HTSE), and thermo-chemical cycles. The example application of the tool was presented for the HES with minimal production of hydrogen ~100000 tonnes/year.

1 INTRODUCTION

Hybrid Energy Systems (HES) are recently a popular research topic, especially considering global trends in increasing efficiency of resource utilization, sustainability, and decarbonization. The HES systems [1], [2] or integrated systems with the concept of Energy Hubs (EH) [3]–[5] can cover the whole ecosystem of technologies coupled to utilize different input energy resources to produce various commodities in an optimized manner. Typically, some sort of power source is the backbone of the system, as electricity has the largest number of applications and future decarbonized perspectives. However, HESs can generate or transform other products, e.g., low-grade heat useful for less demanding industrial processes, cogeneration with district heating, cold, but also high-grade heat for industrial applications, like chemical, metallurgical, and others. HES systems can involve energy storage, batteries, thermal energy storage, and other technologies. It can also involve energy carriers, like alternative liquid or gas fuels, hydrogen or ammonia, etc. These can have applications for the road, public transport, maritime, or air transport industries.

Commonly, in the literature, HESs and EHs are considered as an approach to efficiently integrating Renewable Energy Systems (RES) with other facilities, and unfortunately, nuclear sources are typically omitted without reasonable justification [4], [5]. Introducing nuclear reactors into Nuclear Hybrid Energy Systems (NHES) or clean Energy Hubs can provide a drastic change in their capabilities by providing large electricity or heat sources with highcapacity factors and opening new perspectives for resource utilization. Nuclear reactors can easily be a basis for such systems, and in the literature, there are some examples of proposed solutions for HESs or EHs – see, e.g., Energy Hub proposed for Moorside NPP in the UK [6] or HESs considered for polish industrial sites [2], [7], [8] or coupled reactors with hydrogen production [1], [9], [10].

In this work, we focused on developing a tool to perform optimization of the conceptual design and performance of a generic energy system with coupled heat and electricity sources, mainly nuclear and hydrogen production technologies. The paper presents the current development status, some features, and example applications. The tool is still in the early stage of development.

2 GENERAL PROBLEM DEFINITION

The HES are systems that utilize various input resources to generate several output products, including various forms of energy and energy carriers. The structure of the hypothetical HES considered in this work is presented in Figure 1. The studied energy system is based on electricity and heat generated by a nuclear reactor. For this study, the main product is hydrogen, which is energy carrier. However, also heat and electricity are produced and studied. The inputs to HES are water, imported electricity/heat, and fuel as a primary energy source. The outputs are exports, heat, electricity, and hydrogen outputs but also wastes like carbon dioxide, used water.

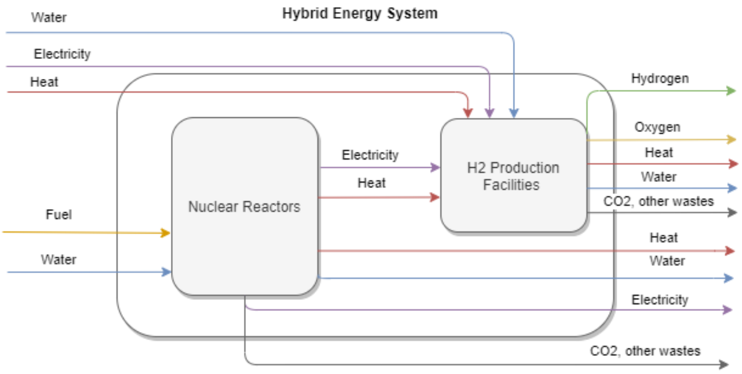

Figure 1: The model of the HES with a nuclear energy source and hydrogen production.

The HES system considered can be described using simply an input-output model, the same way as the EH model ([3]–[5]) is given by the simplest time-independent system of equations Eq. (1).

$$\vec{O} = \bar{\bar{C}} \cdot \vec{I} \quad \xrightarrow{yields} \begin{bmatrix} O_1 \\ O_2 \\ \vdots \\ O_m \end{bmatrix} = \begin{bmatrix} C_{11} & \cdots & C_{1n} \\ \vdots & & \vdots \\ \vdots & \ddots & \vdots \\ C_{m1} & \cdots & C_{mn} \end{bmatrix} \begin{bmatrix} I_1 \\ I_2 \\ \vdots \\ I_n \end{bmatrix} \qquad (1)$$

The basic idea is that there are inputs in the form of a vector $\vec{I}$ and outputs $\vec{O}$, the system transforms the input into output by the transformation matrix $\bar{\bar{C}}$. Inputs and outputs are typically expressed in terms of energy or mass, and the problem is expressed as transformations of these physical quantities. In this work, we expressed all input and outputs in the form of energy or quantities scaled by proper energy-related intensive coefficients.

The basic problem considered in this work was to optimize the given system. The optimization task is trying to find proper energy input, output, and optimal configuration of technologies considering conservation laws (mass-energy conservation), technological, economic, resources, ecology, legal, and safety bounds and constraints. The optimization objectives represent designers' expectations for the desired design, and they are expressed in similar terms as constraints, typically by technical and economic terms but also others – see the idealized problem presentation in Figure 2.

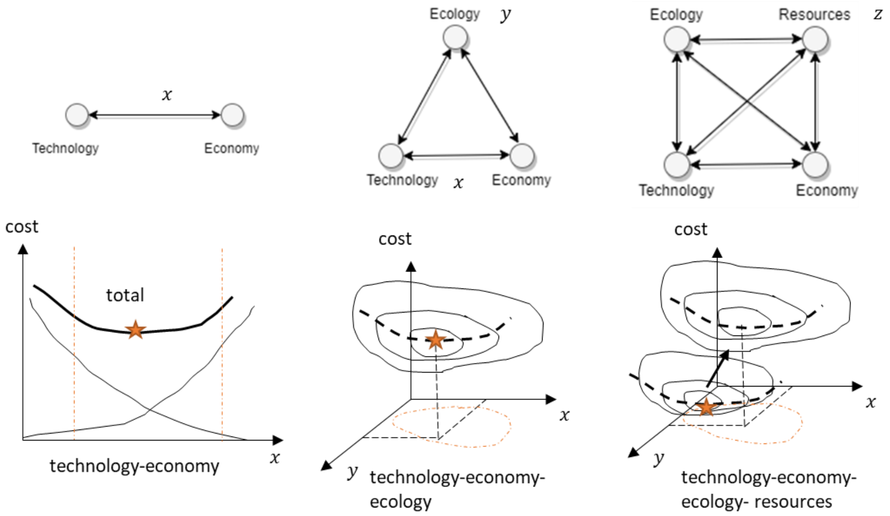

Figure 2: The concept of the engineering optimization problem. Covers optimal solution (star) and the growing number of objectives and constraints (dashed lines) depending on the complexity of the problem arising from left to right. Graph inspired by [12].

For the considered system, Eq. (1) is an elegant mathematical representation, and various more complex models (e.g., with time dependence) can be further developed – see [5], [11]. However, for the studied problem, it is not given as a priori knowledge about the design of HES. Basically, the input and transformation matrix are not exactly known before the solution-finding process. In the studied problem, the optimization algorithm attempts to find implicitly input $\vec{I}$, output $\vec{O}$ and elements of the transformation matrix $\bar{\bar{C}}$, which fulfill the objective, constraints, and bounds defined by the user.

3 DEVELOPED TOOL AND SOLUTION METHODS

The main task considered in this paper was to prepare software that would allow the user to formulate and solve the optimization problem of designing the structure of a Nuclear Hybrid Energy System discussed in the previous chapter. The basic approach was to use MATLAB computational environment with its toolboxes, particularly Optimization Toolbox™ and Global Optimization Toolbox™. The developed tool is basically a communication engine between the user and the MATLAB environment. MATLAB allows the user to formulate optimization problems by the so-called problem-based approach, where the solver is selected automatically by toolboxes, and with the solver-based approach, where the user has control over the solver setup and selection process.

Optimization problems are common in management, economy, and engineering. Many problems can be formulated in a simple linear manner, in the form of the so-called Linear

Programming (also called Linear Optimization, Linear Programming Algorithms) problems, where objectives, constraints, and bounds have linear nature.

The Linear Programming (LP) problem has the following form [13]–[15]:

$$\min_{x} f^T \cdot x \quad such\ that \begin{cases} A \cdot x \leq b \\ A_{eq} \cdot x = b_{eq} \\ lb \leq x \leq ub \end{cases} \tag{2}$$

The solution includes finding an unknown vector x, which minimizes an objective function $f^T \cdot x$. The objective function, in this case, is a linear expression, which is a dot product, where f and x are vectors. The solution vector is subjected to linear inequality constraints ($A \cdot x \leq b$) and linear equality constraints ($A_{eq} \cdot x = b_{eq}$) given by matrices A, A_{eq} and vectors b, b_{eq}. The solution vector is also limited by upper and lower constraints expressed by bounding vectors lb and ub.

In the basic form, vector x can have continuous components. The so-called Integer Linear Programming (ILP) problem introduces into Eq. (2) condition that the vector x components have to be an integer. The Mixed Integer Linear Programming (MILP) allows that some of the components in the vector x are integer, and some are continuous. The integer type problem with two states is a binary problem. The MILP and LP problems are considered in this work as an approach to optimizing HES. In the first case, reactor or electrolyzers can be within a type of series and are not continuous. In the second case, we assume continuous variables. The example applications are presented in the next chapter.

Currently, MATLAB has well-proven capabilities in solving LP-type problems. They can be very efficiently solved with modern solvers (minimizers) – like MATLAB's linprog or intlinprog. It is the case when a single objective function is considered. In the case of multiple objectives, the formulation in Eq. (2) has to be extended to take into account that we have a different objective function; we minimize/maximize more than one objective function. When we have more than one objective function, MATLAB demands the application of more complex solvers. In such a situation, we can use global solvers, e.g., Genetic Algorithm (GA) but also others dedicated to multi-objective optimization problems [15]. In the next chapter, the third example uses multiple objectives and a multiple-objective genetic algorithm solver to find Pareto front solutions.

The approach used in this work and general work logic of the code to solve the problem with a problem-based approach for LP and MILP, is the following:

- Describe and define the problem – using the database.
- Select and create optimization variables
- Define and create an optimization objective or multiple objectives
- Formulate constraints and boundaries – equalities and inequalities
- Execute solution
- Post-process results

The developed tool is prepared with the intention to be object-oriented, and it is currently being developed. The source code is available at the GitLab repository: https://gitlab.com/darczu/pob-hes-h2

4 EXAMPLE PROBLEM DEFINITION

In this paper, three example problems were solved. The LP and MILP problems with single objective function and MILP with multiple objectives. The first two were solved with linprog/intlinprog solvers, and the third was solved with a multi-objective genetic algorithm (gamultiobj).

The industrial facility with nuclear reactors and a generic industrial consumer is postulated (e.g., some chemical facility). The HES provides a supply of low-grade, high-grade heat, hydrogen gas, and electricity to the industrial facility and remaining products can be exported. The task is to find the optimal production of heat, electricity, and hydrogen by each plant in the HES.

For the sake of the test, objective functions are simple, and they consider only monetary cost per energy generation and CO2 production tax. Several other factors must be considered in future investigations. For the problem with a single objective only sum of costs is considered. For multi-objective problems, the same sum is considered, and additionally, the total production of CO2 production is minimized. The example is simplified, so the reader should treat it more as an example academic application of the software.

The HES fulfilling is following assumptions, constraints, and bounds:

- One year is considered, and no time evolution is considered. It covers year-averaged values of inputs and outputs.
- Minimum hydrogen production is 100000 tH2/year = 3.171 kgH2/s – main assumption.
- The minimum average low-grade heat and high-grade heat production are 500 MWth/250MWth, and the maximum is 2000 MWth/10000MWth (effectively unlimited). Waste heat is also treated here as low-grade heat.
- Minimum/Maximum average electricity production is 500 MWe/1000MWe
- Nuclear technologies PWR unit size 1000 MWe, 33% efficiency with CF=90%; HTR reactor with unit size 250 MWe, 40% efficiency and CF=80%. Also, a 300 MWe, CF=0.8, efficiency 45%, coal plant is added – totally three technologies. Only one coal plant unit is allowed.
- Hydrogen generation technologies – only Low-Temperature Electrolysers are considered in the example: alkaline (AEK) and proton-exchange (PEM) electrolyzers with a type of series for AEK 20 and 10 MWe and PEM with 25, 15, and 5 MWe – totally five technologies.
- Energy is conserved. The import of electricity, heat, or hydrogen is not considered (forced zero). The heat and electricity generated are consumed or exported.
- PWR reactors cannot produce high-grade heat; only coal and HTR plants have this capability (in this example).
- Carbon tax is assumed ~50$/tCO2.

Three main groups of optimization variables are considered. These are nuclear sources production (9 variables), hydrogen technology consumption (15 variables), import/export (6 variables) of electricity, low-grade heat, and high-grade heat. The next two optimization variables are the integer number of units for the nuclear plant (3 variables) and hydrogen plant (5 variables), and this variable work only for the mixed-integer problem. Totally for MILP, it is 38 optimization variables, and for LP, it is 30 variables. The data, technology, and costs for electrolyzers and reactors are based on [1] and some generic data.

5 RESULTS AND DISCUSSION

The solution of the LP and MILP with a single objective takes less than <1.5 seconds. In the case of MILP, multi-objective solved with GA takes <350 seconds. The comparison of results for three considered examples is presented in Table 1. The first solution is a simple tuning of input/output energy rates to find an optimal solution and fulfill the criteria. In two other cases, it is limited by the type of series for devices, and different solutions are found.

For hydrogen technologies, the dominating solution is AEK 10MWe which is the cheapest, but also PEM 15 MWe is comparable. In effect, for MILP solutions, combination of these two units is found to match production demand. For LP, only AEK 10MWe is selected as the cheapest. In all cases, only slightly above 100ktH2/year are produced.

In the case of single objective MILP, the solver selected 1xHTR, 1xPWR, and 1xCoal plant. HTR produces the lowest amount of CO2, it is the most expensive, coal produces a lot of CO2 but is the cheapest energy, and PWR is an intermediate in terms of carbon cost and energy cost.

In the case of MILP, with multiple objectives, 18 different solutions were found, forming the Pareto front. The solution with 1xHTR, 1xPWR, and 1xCoal was selected in seven solutions in the set. Totally among all solutions, three different options were found – 6xHTRs only; 1xPWR, 1xHTR, 1xCoal, and a system with 2xHTRs, 1xPWR. Hence, there is no single simple answer for the problem in the form as it was formulated. Table 1 (last column) shows details of solution number 2 with PWR+HTR+Coal, which is similar to the MILP solution for one objective. Final parameters are effectively equivalent, with the exception being a slightly different set of electrolyzers. For MILP problems, very similar export conditions are predicted.

Table 1: Example results for LP and MILP with a single objective and MILP with multiple-objective optimization.

Case/Parameter	Device type	LP – single objective	MILP – single objective	MILP – multi objective Pareto with 18 solutions example no.2
Nuclear production (MJ/s): electricity/low-grade /high-grade heat	PWR:	544.5/1105.5/0	1000/2030.3/0	999.9/2030.3/0
	HTR:	132.3/0/161.7	250/0/305.5	250/1.0/304.5
	Coal:	300/0/338.3	300/143.8/194.4	299.9/139.8/198.5
Hydrogen dedicated energy consumption (MJ/s): electricity/low-grade heat/high-grade heat	AEK 20MW:	0/0/0	0/0/0	0/0/0
	AEK 10MW:	576.8/86.9/0	550/82.8/0	569.9/85.9/0.00012
	PEM 25MW:	0/0/0	0/0/0	0/0/0
	PEM 15MW:	0/0/0	30/3.9/0	0/0/0
	PEM 5MW:	0/0/0	0/0/0	9.99/1.37/0.03
Export of energy (MJ/s): electricity/low-grade /high-grade heat	Export:	200/518.6/250	770/1587.3/250	769.99/1583.92/252.9
# Nuclear units	PWR/HTR/Coal	continuous	1/1/1	1/1/1
# Hydrogen units	AEK: 20/10/… PEM: /25/15/5	continuous	0/55/0/2/0	0/57/0/0/2

6 CONCLUSIONS AND SUMMARY

The early version of the software for optimization of the Nuclear based HES for hydrogen production was developed. It was presented that it has applicability in solving optimization problems for Linear Programming, Mixed Integer Linear Programming with single and multiple objectives. The tool will be further developed in order to study various options for HES with nuclear-based hydrogen generation and likely other applications. The tool will be soon available at the GitLab open-repository: https://gitlab.com/darczu/pob-hes-h2

In this paper, we focused on standard Linear Programming and Mixed Integer Linear Programming problems. These are very common and popular to formulate and solve this kind of optimization problem. Of course, this approach has some limitations, and also MATLAB has its own limitations. More advanced and more developed tools dedicated to similar applications are available in the literature, e.g., the Python-based Calliope package [16]–[18]. It can be used to solve MILP and LP problems for complex energy systems at the scale of a country using powerful solver packages like Gurobi. However, the standard Calliope release currently does not allow multiple objectives, and MATLAB Global Optimization Toolbox^{TM} easily allows it. In spite of that, further planned work will also cover Calliope applications in the framework of the considered project.

7 ACKNOWLEDGMENT

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