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# A multi-period optimization model for the design of mass networks including conversion systems and gas storage models: application for hydrogen generation, distribution and storage

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#### Abstract

- <sup>10</sup> A multi-period mixed-integer-linear-programming problem for the design of mass networks is proposed in this paper. Design of mass networks, conversion systems and storages is done so as to minimize the capital expenses and operating costs and fulfill demand in resources. This work provides a detailed model of compressed gas storage, considering pressure state inside gas tank, compres-
- <sup>15</sup> sion costs and compressor design, which have not been considered before in a linear model, with a discrete pressure scale. The performance of the model is assessed on a hydrogen network design problem, including renewable electricity, electrolyzer design and hydrogen storage. The share of renewable electricity use increases from 60% to 90% with hydrogen storage. Different compressed gas
- storage linearized models are compared with different pressure scales and the linearization error is assessed. The introduction of discrete intermediate pressures reduces the committed error on compressor power and operating costs, due to the linearization.

Keywords: MILP, multi-period, hydrogen network, compressed gas storage,

25 electrolyzer

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# Highlights

- A multiperiod MILP problem is developed for the optimal design of hydrogen network and storage.
- A new linearized compressed gas storage model is proposed, considering compression energy costs.
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- A discretized pressure scale is introduced.
- Comptutational and precision performances are assessed on a case study.

# 1. Introduction

#### 1.1. Context

- The share of renewable resources in final energy consumption is increasing in Europe since 2004 and a target of 32% is set by 2030 (Eurostat, 2020). In this way, design and development of multi-energy systems appear to be an opportunity. They consist of the integration between several energy networks of different nature: electricity, gas, heating and cooling. These energy sectors are traditionally designed separately even though close interactions can take
- place. For instance, technologies such as heat pumps, Combined Heat and
  Power (CHP) or gas turbines couple heat and electricity networks. Heat pumps
  consumes electricity and can supply energy to a heat network while CHP can
  produce both electricity and heat. Moreover, one of the main drawbacks of re-
- <sup>45</sup> newable electricity (wind, photovoltaic) is their intermittency. They are hardly monitored, their production must be used instantaneously and matching electricity supply and demand is mandatory. The utilization of electric storages like lithium-ion batteries can be a solution but they are mainly short-term solutions (Kusko and DeDad, 2005; Smith et al., 2008; Walker et al., 2016). They hardly
- store electricity for a long-period and it requires costly investments in case of seasonal storage. The power-to-gas technologies can also tackle this issue. The idea is to convert electricity into gas. The surplus of electricity from renewable resources can be converted into hydrogen ( $H_2$  conversion by electrolyzer)

and into natural gas (methanation). Moreover, the conversion into natural gas

<sup>55</sup> benefits the already existing distribution gas networks and storages. Actually, the total world gas storage capacity exceeds largely the total world power from wind and solar (Götz et al., 2016), thus, power-to-gas can provide flexibility and enhance the integration of renewable intermittent resources, using gas as an energy carrier. Actually, hydrogen is characterized by a high energy den<sup>50</sup> sity (three times higher than liquid hydrocarbon based fuels) and low losses in transportation, thus it is seen as an efficient energy carrier (Walker et al., 2016;

# Mazloomi and Gomes, 2012).

# 1.2. Hydrogen production

Hydrogen can be produced through several pathways. The most popular
is steam-methane reforming (SMR) (almost 48% of total hydrogen production (Mazloomi and Gomes, 2012)) from fossil fuels but it generates greenhouse gases (CO, CO<sub>2</sub>). This pathway produces non-renewable hydrogen, generally referred as 'grey hydrogen'. The other pathway is water electrolysis, providing a high purity of hydrogen and is considered to be a promising technology to mass
produce hydrogen (Walker et al., 2016). The water is decomposed into oxygen and hydrogen by means of a continuous electric current supplied by a power source, a battery or a cell, connected by electrodes to the water. The electricity can be produced by renewable resources (wind or solar) making the hydrogen renewable (and called 'green hydrogen'). The main reactions are equations (1)
to (3):

$$H_2O + \text{Electricty} \longrightarrow H_2 + \frac{1}{2}O_2$$
 (1)

Reduction at the cathode: 
$$2H^+ + 2e^- \longrightarrow H_2$$
 (2)

Oxidation at the anode: 
$$H_2O \longrightarrow 2H^+ + 2e^- + \frac{1}{2}O_2$$
 (3)

Two main types of electrolyzers are used: alkalyne electrolyzers and Polymer Electrolyte Membrane (PEM) electrolyzers (Abdin et al., 2015, 2017). Al-

- kalyne water electrolysis is the most used in industry nowadays because they are cheaper. However, hydrogen produced from PEM has some advantages: the hydrogen produced is highly pure and there are no hazardous chemicals contrary to alkalyne electrolyzers. Moreover, they can reach higher current density values, above 2 A/cm<sup>2</sup>, improving the yield and its profitability. Finally, they
- can also operate in a large power range, from 10% to 100% of the nominal power or even higher (Barbir, 2005; E&E Consultant et al., 2014). Different degrees of complexity can be found in literature about PEM electrolyzer modelling. The first PEM models of electrolyzer were published from 2002 and focused on steady-state behavior (Onda et al., 2002; Khan and Iqbal, 2005; Busquet et al.,
- 2004; Kélouwani et al., 2005; Görgün, 2006). However, given the intermittency and the variability of renewable power sources, dynamic behavior should be taken into account for detailed model. Dynamic behaviour consideration requires more comprehensive models, including differential equations, thus their resolution increases the model complexity (Falcão and Pinto, 2020; Carmo et al.,
- <sup>95</sup> 2013; Olivier et al., 2017). Dynamic model of PEM has been studied in the literature (Abdin et al., 2017; Carmo et al., 2013; Olivier et al., 2017; Marangio et al., 2011; Lebbal and Lecœuche, 2009; Nie et al., 2009; Nie and Chen, 2010; Awasthi et al., 2011; García-Valverde et al., 2012; Gabrielli et al., 2016). These theoretical models are in most cases confronted to experimental data. They
- take into account activation losses, based on Butler-Volmer kinetic laws (Abdin et al., 2017; Marangio et al., 2011; Lebbal and Lecœuche, 2009). Recently Falcão and Pinto (2020) presented a review of PEM electrolyzers modelling, detailing the technology basic principles. PEM modelling improves the understanding of the electrolyzer and helps the prediction of their behaviour. However, due to
- <sup>105</sup> model complexity, simpler models are often used in large-scale energy problems, like power-to-gas problems (Reuß et al., 2019). Electrolyzers are defined by its efficiency, most of the time static and independent of operating conditions. Its efficiency relates of the conversion of water into hydrogen and oxygen, with

electricity. In Kélouwani et al. (2005); Zervas et al. (2008), the electrolyzers is modelled using conversion factors, directly provided by the manufacturers and a comparison between simulation and experiments are conducted.

#### 1.3. Hydrogen in supply chain design

Electrolyzer modelling is also covered in hydrogen supply chain design topics
(Li et al., 2019; Yue et al., 2014; Moreno-Benito et al., 2017; Van Den Heever and Grossmann, 2003; Martín and Grossmann, 2011). Almansoori and Shah (2006, 2009) presented an optimization model of a future hydrogen supply chain. This model was first static and then extended to multiperiod (long term evolution and infrastructure design). Production pathways and transportation networks were
optimized under the economic aspect. Li et al. (2020) developed a MILP model of a hydrogen supply network. Feedstock supply (from SMR, electrolysis and biomass gasification), production facilities and transportation were considered to minimize the cost of hydrogen. The model was static and did not consider hydrogen storage. Also, Chahla and Zoughaib (2019) developed a methodol-

- ogy for the integration of biomass conversion into a hydrogen energy system in a non-cooperative governance, where the industrial actors search to maximize their own interest. The model was also static and without hydrogen storage. Samsatli and Samsatli (2015) developed a MILP model to design the hydrogen network considering hourly hydrogen demand and electricity from wind tur-
- bines. Different conversion technologies, modelled by a conversion factor were modelled in order to supply hydrogen. Different type of storages can also be used: underground, compressed gas at 200 bars, liquid and metal hydride. A non uniform time discretization is used in order to address the tractability challenge. Most of papers tackling the multiperiod problem of hydrogen demand
- and the variability issue of renewable resources integrate compressed hydrogen storage. This is one of the most mature technology for hydrogen storage compared to metal hydride and cryogenic (Barthelemy et al., 2017). In these papers, compression costs are included in the storage cost but this cost is independent

of the pressure inside the storage (Kélouwani et al., 2005; Zervas et al., 2008;
Almansoori and Shah, 2009; Samsatli and Samsatli, 2015; Ruiming, 2019) and it does not allow compressor design. As far as the authors know, the question of designing the compressor for storages is barely considered in power-to-gas topics and it has not been considered yet in a linear model.

This should be considered because:

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- The investment cost of a compressed storage depends also on the size (power) of the compressor.
- The compression mass flow depends on compressor sizing. Mass flow is limited to its maximal power.
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• The compression energy need depends on pressure changes, thus operating costs depend on pressure changes.

• Computing compression energy consumption allows us to estimate compressor cooling, thus estimate the recoverable waste heat potential.

However, the equations describing the behaviour of compression gas storages
<sup>155</sup> are non-linear, particularly the equation of state and the computation of work compression. This adds to the difficulties in solving by reducing the computational tractability, which explains the lack of compression modelling.

# 1.4. Goal of this paper

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Therefore, this paper proposes a linearized model of compressed gas storage based on a pressure discretization. This model is included into a multi-period optimization problem for the design of mass and energy networks, extending the work of Ghazouani et al. (2017). Generic models of conversion systems are also included in the model. A Mixed-Integer-Linear-Programming (MILP) problem

<sup>165</sup> is defined in order to design storages, conversion systems and networks considering mass and energy demand. The objective function is the minimization of the total costs (investment and operating costs). The problem is applied to a hydrogen case study, inspired of Samsatli and Samsatli (2015).

#### 1.5. Structure of paper

- This paper is structured as follows. The problem statement is presented in section 2 and the equations of the MILP problem are detailed in section 3. Finally, the model is applied to a hydrogen case study in section 4. It deals with a hydrogen demand, varying in time. The hydrogen demand is fulfilled thanks to an electrolyzer using electricity produced by wind turbines and the grid. The compressed hydrogen storage linear model is also used. An evaluation of the
- approximation error due to the linearization is done. Some perspectives of the current work are presented in section 5.

# 2. Problem statement

#### 2.1. Superstructure definition

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This paper presents a multi-period optimization model for the design of multi mass networks, conversion and storage systems between different clusters. Each cluster represents an industrial actor and can exchange resources (energy, water, hydrogen, ...) through mass networks to other clusters of the territory. Each cluster  $c \in C$  can contain different elements:

- Process sources  $(j_r \in J_p)$ . They correspond to material resources (ex: H<sub>2</sub>) or effluents (ex: water) that are available and can be reused in the process or in the territory. They are defined by their type  $r \in \mathcal{R}$ , a given mass flow rate  $L_{c,j_r,t}$  for each period of time  $t \in \mathcal{T}$ .
  - Process sinks (i<sub>r</sub> ∈ I<sub>p</sub>). They correspond to process units that require a given mass flow rate (G<sub>c,i<sub>r</sub>,t</sub>) for each material type r ∈ R and each period of time t ∈ T.
  - Variable sources  $(j_r \in J_v)$  are available in a cluster in order to satisfy process sink requirements. Their mass flow rate  $L_{c,j_r,t}^v$  are unknown for

each material type  $r \in \mathcal{R}$  and each period of time  $t \in \mathcal{T}$ . They are variables to be optimized. They represent the input flow of systems such as storages, conversion systems or the purchase of a resource, with an associated cost.

- Variable sinks (i<sub>r</sub> ∈ I<sub>v</sub>) are available in a cluster in order to discard resources that cannot be used directly in a cluster. Their mass flow rate G<sup>v</sup><sub>c,i<sub>r</sub>,t</sub> are unknown for each material type r ∈ R and each period of time t ∈ T. They are variables to be optimized. They represent the output flow of systems such as storages, conversion systems or resource disposal at a certain cost.
- <sup>205</sup> More sophisticated systems can be defined, based on the definition of sources and sinks:
  - Mass storages (s<sub>r</sub> ∈ S), created by the association of a variable source and sink ((j<sub>r</sub>, i<sub>r</sub>) ∈ J<sub>v</sub> × I<sub>v</sub>). They can be daily or seasonal storages. They are characterized by capital and operating costs. This element is described further in details in 3.3.
  - Conversion systems (sc ∈ SC), created by the association of variables sources and sinks ((j<sub>r</sub>, i'<sub>r</sub>) ∈ J<sub>v</sub> × I<sub>v</sub>). They are used to convert resources in other resources (for example: electrolyzer and H<sub>2</sub>), with an electrical demand or production. This element is described further in details in 3.5.
- Resources can be exchanged inside a cluster (between different sinks, sources and technologies) or between different clusters through a dedicated mass network. This network is characterized by an investment cost (proportional to the length of a path).

#### 220 2.2. Optimization target

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The target of the study/analysis is to determine optimal results for:

- The mass flow rate between the different sources and sinks (inside a cluster or between different cluster);
- the network topology ;
- the storage evolution with time ;
  - the mass storage design ;
  - the conversion systems design ;
  - the investment decisions such as the localization of different technologies.

So as to minimize the Total Annualized Costs (CAPEX+OPEX) while sat-230 isfying the resource needs of each cluster in a territory.

# 3. Model formulation

#### 3.1. Mass balance inside a cluster

Inside each cluster  $c \in C$ , the mass flow requirement  $G_{c,i_r,t}$  of each sink  $i \in I$ has to be met for a sink  $i_r$  (equation (4)) and for a variable sink  $i_r$  (equation (5)):

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$$\forall t \in \mathcal{T}, \forall i_r \in I_p, \forall r \in \mathcal{R} \quad G_{c,i_r,t} = \sum_j L_{c,ij_r,t} + \sum_j L_{c,ij_r,t}^v$$
(4)

$$\forall t \in \mathcal{T}, \forall i_r \in I_v, \forall r \in \mathcal{R} \quad G_{c,i_r,t}^v = \sum_j L_{c,ij_r,t} + \sum_j L_{c,ij_r,t}^v$$
(5)

where  $L_{c,ij_r,t}$  is the mass flow from a source  $j_r$  to the sink  $i_r$  and  $L_{c,ij_r,t}^v$  is the mass flow from a variable source  $j_r$  to the sink  $i_r$ .

In the same way, the mass flow leaving a source  $j_r$  (equation (6)) and a variable source  $j_r$  (equation (7)) is equal to its total flow rate:

$$\forall t \in \mathcal{T}, \forall j_r \in J_p, \forall r \in \mathcal{R} \quad L_{c,j_r,t} = \sum_i L_{c,ij_r,t} + \sum_i L_{c,ij_r,t}^v \tag{6}$$

$$\forall t \in \mathcal{T}, \forall j_r \in J_v, \forall r \in \mathcal{R} \quad L_{c,j_r,t}^v = \sum_i L_{c,ij_r,t} + \sum_i L_{c,ij_r,t}^v$$
(7)



Fig. 1. Superstructure for mass balance in a cluster.

Figure 1 represents the superstructure and the mass balance inside a cluster between sources and sinks.

## 3.2. Mass networks

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Exchange of material between industries, modelled by the clusters, is realized through mass networks. A mass network  $(j_r, i_r) = m \in M_{net}$  of a resource  $r \in \mathcal{R}$  is modelled as a variable source  $j_r \in J_v$  and a variable sink  $i_r \in I_v$  inside each cluster  $c \in \mathcal{C}$  of the problem. We note  $c_m \in \mathcal{C}_m$  the subset of clusters interacting with the mass network m. The variable source represents the matter provided by the network to the cluster and the variable sinks represent the mat-250 ter leaving the cluster and entering into the network. Therefore, mass exchange

between a cluster and a mass network are defined by the set of equations (4)to (7). Specific equations for the mass network are defined.

We assume that there is no mass accumulation in the network : the matter entering into the network is instantaneously consumed by a cluster (equation (8)): 255

$$\forall t \in \mathcal{T}, \forall (j_r, i_r) = m \in M_{net}, \sum_{c \in \mathcal{C}_m} G_{c, i_r, t}^v = \sum_{c \in \mathcal{C}_m} L_{c, j_r, t}^v$$
(8)

A mass network m is defined by a certain number of authorized paths  $p_m \in$ P, connecting two clusters. To each path  $p \in P$  is associated an arbitrary direction  $\delta_p = \pm 1$ , orienting the path. We define also the set  $\mathcal{P}_c$  corresponding



Fig. 2. Illustration of a mass network

to the all paths passing through a cluster c:

$$\forall t \in \mathcal{T}, \forall c \in \mathcal{C}, \sum_{p \in \mathcal{P}_c} L_{p,t}^{path} \delta_p = G_{c,i_r,t}^v - L_{c,j_r,t}^v \tag{9}$$

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Where  $L_{p,t}^{path}$  is the flow rate (which can be positive or negative depending on the orientation of the path) through the path p at the time t (figure 2 and equation (9)) is applied to each cluster.

For example, in figure 2, three clusters are present, and one mass network connects each them. Three paths are possible: from C1 to C2  $(p_1)$ , from C1 to C3  $(p_3)$  and from C2 to C3  $(p_2)$ .  $G^v f_{c,i_r,t}$  is the mass flow entering into the network at the cluster  $c_1$  (or leaving the cluster  $c_1$  through a waste sink) and  $L_{c,i_r,t}^v$  is the mass flow leaving the network at the cluster  $c_1$  (or entering into the cluster  $c_1$  through a fresh source).

Binary variables are introduced in order to detect whether a path is used in a mass network through big-M equations (equations (10) and (11)):

$$\forall p \in \mathcal{P}, \forall t \in \mathcal{T}, L_{p,t}^{path} - \Omega \cdot b_p \le 0$$
(10)

$$\forall p \in \mathcal{P}, \forall t \in \mathcal{T}, L_{p,t}^{path} + \Omega \cdot b_p \ge 0$$
(11)

where  $\Omega$  is a great number (the maximum capacity of the paths for example)

#### 3.3. Mass storage formulation

Mass storage  $((i_r, j_r) = s_r \in S)$  is modelled by a couple of a variable sink  $j_r$ and of a variable source  $i_r$  for the resource r in a cluster c. We define the sets  $I_s$  and  $J_s$  corresponding to the subsets of variables sources and sinks belonging to a storage. The storage is modelled by three main positive variables: the flow entering the storage  $G_{c,j_r,t}^v$ , the output flow  $L_{c,i_r,t}^v$  and the amount of mass stored at the end of the period  $S_{c,s_r,t}$ . We assume that the steady state is established at each period.

The storage evolution is given by equation (12) where  $\delta t_t$  corresponds to the duration of a period  $t \in \mathcal{T}$ :

$$S_{c,s_r,t+1} = S_{c,s_r,t} + \left(G_{c,j_r,t}^v - L_{c,i_j,t}^v\right) \cdot \delta t_t \quad \forall (i_r, j_r) = s_r \in S, \forall t \in \mathcal{T}$$
(12)

The maximum capacity of a storage is given by equation (13):

$$Max_{-}S_{c,s_{r}} \ge S_{c,s_{r},t} \quad \forall (i_{r},j_{r}) \in S, \forall t \in \mathcal{T}$$

$$(13)$$

Big-M formulation are used in order to define binary variables (equations (14) and (15)), defining the existence of inlet and outlet flows:

$$G_{c,j_r,t}^v \le b_{c,j_r,t}^{in} \cdot \Omega \quad \forall j_r \in J_s, \forall t \in \mathcal{T}$$

$$\tag{14}$$

$$L_{c,i_j,t}^v \le b_{c,i_r,t}^{out} \cdot \Omega \quad \forall i_r \in I_s, \forall t \in \mathcal{T}$$

$$\tag{15}$$

Emptying or filling a mass storage simultaneously is forbidden (equation (16)):

$$b_{c,i_r,t}^{out} + b_{c,j_r,t}^{in} \le 1 \quad \forall s_r = (i_m, j_m) \in S, \forall t \in \mathcal{T}$$

$$(16)$$

A binary is used to detect if a mass storage  $(i_r, j_r)$  is used (equation (17)):

$$Max\_S_{c,s_r} \le b^S_{c,s_r} \cdot \Omega \quad \forall s_r \in S$$

$$\tag{17}$$

## 3.4. Compressed gas storage

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# 290 3.4.1. Limitations of the incompressible storage model

The equations presented above (equations (12) to (17)) are adapted for incompressible mass storage. They are not sufficient to model compressed gas storage:

- The discharge pressure impacts the compression work, thus the operating costs.
- The power input of the compressor depends on the intake flow and on the discharge pressure.
- The investment cost of a compressed gas storage depends on the nominal power of the compressor
- Therefore, an extended model is proposed in this paper in order to consider the gas compressibility, the compressor design and evaluate the compression costs. This model includes the computation of the gas pressure inside the storage, the volume design and the energy demand for the gas compression. We define the subset  $S_g \subset S$  corresponding to the set of compressed gas storage. The main assumptions are:
- 1
  - The gas is an ideal gas, with a constant heat capacity ratio  $\gamma.$
  - The gas is compressed by a multi-stage compressor with intercooling.
  - The pressure ratio is identical for all the stages (and depends on the number of stages).
- The temperature  $T_{s_g}$  inside the storage is constant.

The mechanical power needs for the compression per mass flow rate  $w_{s_g}$  is expressed by equation (18):

$$w_{s_g} = \frac{NR\gamma T}{M\left(\gamma - 1\right)} \left( \left(\frac{P_{s_g}}{P_1}\right)^{\frac{\gamma - 1}{N\gamma}} - 1 \right) \quad \forall s_g \in S_g \tag{18}$$

where N is the number of compression stages,  $P_1$  is the pressure at the inlet and  $P_{s_g}$  is the pressure inside the storage.

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The highest pressure inside the storage can be found through the application of the ideal gas law:

$$P_{s_g}V_{s_g} = \frac{Max\_S_{c,s_g}}{M_g}RT_{s_g} \quad \forall s \in S_g$$
<sup>(19)</sup>

These two equations (18) and (19) are non-linear because of the presence of the power function and because of the multiplication of several variables <sup>320</sup> between them: pressure, volume and the mass flow rate. Linearization of these equations are developed in section 3.4.2.

#### 3.4.2. Mathematical linearized model

A pressure discretization is introduced: each compressed gas storage is defined by a pressure scale and equation (18) is pre-computing on each pressure <sup>325</sup> interval. The mean value is used for pre-computed the mechanical compression work on each interval (equation (20)). Figure 3 presents and compares the value for the evolution of mechanical compression according to the pressure inside the storage (assuming the gas is hydrogen and there are four compression stages) with the discrete mean values computed by equation (20). This discretization

- can drive to another approximation. The pressure inside the storage can vary during a time step, leading to a shift for the discrete pressure between two consecutive time steps and the mean value used can be far from the actual value. Therefore, the computation of the mechanical work will consider two consecutive time steps in order to reduce this approximation. Depending on the
- pressure inside the storage, the corresponding mean value will be used. Indeed, the pressure inside the storage can be under or over-estimated, that can lead to errors in the computation of work. Thus, a trade-off is necessary between the

discretization and the accuracy level.

$$\widetilde{w_{c,s_g,p}} = \frac{1}{P_{p+1} - P_p} \int_{P_p}^{P_{p+1}} \frac{NR\gamma T}{M(\gamma - 1)} \left(\frac{p}{P_1} \frac{\gamma^{-1}}{N\gamma} - 1\right) dp$$

$$\forall s_g \in S_g, \forall p \in \{P_0, P_1, \cdots, P_{N_{s_g} - 1}\}$$

$$(20)$$



(a) 1 pressure interval

(b) 2 pressure intervals



(c) 3 pressure intervals

Fig. 3. Discretization of the mechanical work for compression

The superstructure for the compressed gas storage is presented in figure 4: the gas volume is fictively divided in several storages with the same volume and with the same amount of gas stored. Each fictive storage is defined by its own pressure interval and a dedicated flow rate. Binary variables are then introduced for each fictive storage and are used to determiner which pressure interval and which fictive storage are used. In other words, this binary is equal to 1 if the pressure inside the storage corresponds to this fictive storage.



Fig. 4. Superstructure for the compressed gas storage.

The mass flow rate entering the storage is hence discretized through the pressure discretization for two consecutive time steps (subscript before/after) (equations (21) to (24)):

$$G_{c,i,t}^{v} = \sum_{p_s \in P} L_{c,s,t,p_s}^{p,in,before} \quad \forall t \in \mathcal{T}, \forall (i,j) = s \in S_g$$

$$(21)$$

$$G_{c,i,t}^{v} = \sum_{p_s \in P} L_{c,s,t,p_s}^{p,in,after} \quad \forall t \in \mathcal{T}, \forall (i,j) = s \in S_g$$
(22)

$$L_{c,s,t,p_s}^{p,in,before} \le \Omega \cdot bin_{s,t,p}^P \quad \forall t \in \mathcal{T}, \forall s \in S_g$$
(23)

$$L_{c,s,t,p_s}^{p,in,after} \le \Omega \cdot bin_{s,t+1,p}^P \quad \forall t \in \mathcal{T}, \forall s \in S_g$$
(24)

$$\sum_{p \in P} bin_{s,t,p}^{P} = 1 \quad \forall t \in \mathcal{T}, \forall s \in S_{g}$$
(25)

The energy required at the compressor is computed using the two pressure <sup>350</sup> states before and after filling the storage with gas in order to consider pressure changes (equation (26)):

$$\widetilde{w}_{s,t}^{comp} = \sum_{p \in P} \widetilde{w}_{c,s,t,p} = \frac{1}{2} \sum_{p \in P} L_{c,s,t,p_s}^{p,in,after} \widetilde{w_{c,s,p}} + \frac{1}{2} \sum_{p \in P} L_{c,s,t,p_s}^{p,in,before} \widetilde{w_{c,s,p}}$$

$$\forall t \in \mathcal{T}, \forall s \in S_g$$

$$(26)$$

Big-M constraints are introduced in order to identify the pressure interval inside the storage, via the ideal gas law (equation (27)).  $S_{c,s,t}$  is the total amount stored,  $V_s$  is the volume of the storage and  $\Omega$  is a great number. If  $bin_{s,t,p}^P = 1$ during a time step, the amount of mass is restricted by the two equations (right hand side of the equations), the pressure inside the storage belongs to the  $p^{th}$ interval, the corresponding mean value of compression energy is used and the ideal gas law can be applied. When  $S_{c,s,t}$  reaches an infimum or supremum defined by the RHS of equation (27), the pressure interval changes.

$$S_{c,i_{m},j_{m},t} \geq \frac{pV_{i_{m},j_{m}}}{M_{m}RT_{i_{m},j_{m}}} - \left(1 - bin_{i_{m},j_{m},t,p}^{P}\right) \cdot \Omega$$

$$S_{c,i_{m},j_{m},t} \leq \frac{pV_{i_{m},j_{m}}}{M_{m}RT_{i_{m},j_{m}}} + \left(1 - bin_{i_{m},j_{m},t,p}^{P}\right) \cdot \Omega$$

$$\forall t \in \mathcal{T}, \forall (i_{m},j_{m}) \in S_{g}, \forall p \in P$$

$$(27)$$

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The storage volume is designed by equation (28), using the minimum of gas stored at the lowest pressure and by the maximum of gas stored at the highest pressure (equation (28)).

$$Max\_S_{c,s} = \frac{P_{s,N_s}V_s}{RT_s} \quad \forall s \in S_g$$

$$Min\_S_{c,s} = \frac{P_{s,0}V_s}{RT_c} \quad \forall s \in S_g$$
(28)

The nominal power of the compressor is computed by the equation

$$P_s \ge \widetilde{w}_{s,t}^{comp} \quad \forall t \in \mathcal{T}, \forall s \in S_g$$
(29)

#### 3.5. Conversion system formulation

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Conversion systems consist of process that convert resources (electricity, material) into other resources. They are modelled and introduced into the problem.



Fig. 5. Representation of a generic conversion system.

The concept of sinks and sources is re-used for their modelling. A schematic representation of a conversion system is presented on figure 5. For each conversion system  $(i, j) = cs \in CS$  is associated a number  $N_i$  of variable sinks

- (resource input), a number  $N_j$  of variable sources (resource production) and electrical power is associated to the conversion (positive or negative, depending if the conversion system generates or consumes electricity). The mass flow rates and electrical power are variables of the system, to be designed. We define also the subsets  $I_{cs}$  and  $J_{cs}$  corresponding to the sinks and the sources associated
- to a conversion system *cs*. For example for an electrolyzer, as used in the case study 4, water and electricity will be the variable sinks while hydrogen and oxygen will be the variable sources of the conversion system.

The behaviour of the conversion system in nominal mode can be represented by a generic linear function, linking all the variables of the system (equation (30)):

$$\forall t \in \mathcal{T}, F\left(L_{c,j,t}^{v}, G_{c,i,t}^{v}, P_{cs,t}\right) = 0$$
(30)

The conversion system is modelled as a grey box and is characterized by different ratio between a reference source  $j_f$  and the other sources j and sinks i:

$$L_{c,j,t}^{v} = rs_j L_{c,j_f,t}^{v} \quad \forall t \in \mathcal{T}, \forall j \in J_{cs}$$

$$(31)$$

$$G_{i,t}^{v} = rs_i L_{c,j_f,t}^{cs} \quad \forall t \in \mathcal{T}, \forall i \in I_{cs}$$

$$(32)$$

<sup>385</sup> The power consumption or generation of the conversion system is given by

equation (33):

$$P_{cs} \ge P_{cs,t} \quad \forall t \in \mathcal{T}, \forall cs \in CS \tag{33}$$

A binary variable is also defined in order to detect the use or not of the conversion system (equation (34)):

$$P_{cs} \ge \Omega b_{cs} \quad \forall cs \in CS \tag{34}$$

## 3.6. Electricity balance

Electricity consumption and production of each cluster is also taken into account. The electricity consumption  $EC_t$  is aggregated from the consumption of the compressed gas storage  $S_g$  and the conversion systems consuming electricity  $SC_c$ .

$$EC_t = \sum_{s \in S_g} \widetilde{w}_{s,t}^{comp} + \sum_{sc \in SC_c} P_{sc,t} \quad \forall t \in \mathcal{T}$$
(35)

The electricity production  $EP_t$  is aggregated from the electrical sources in <sup>395</sup> all the clusters and form the conversion systems generating electricity  $SC_p$ 

$$EP_t = \sum_{c \in \mathcal{C}} EP_{c,t}^c + \sum_{sc \in SC_p} P_{sc,t} \forall t \in \mathcal{T}$$
(36)

The electricity balance is achieved at the territory scale. Each cluster is connected to the grid and can buy electricity from it if necessary (equation (37)), with a limitation (equation (38)).

$$EP_t + EP_t^{res,in} = EC_t + EC^{res,out} \quad \forall t \in \mathcal{T}$$
(37)

$$EP_t^{res,out} \le EP_t^{limit} \quad \forall t \in \mathcal{T}$$
 (38)

## 400 3.7. Objective Function

The objective function is the minimization of the total actualized cost (TAC) including the investment costs CAPEX and the operational costs OPEX (equation (39)), assuming an actualization ratio  $r_a$  and a number of operating years

 $N_y$ :

$$\min\left(CAPEX + \sum_{y=1}^{N_y} \frac{OPEX}{\left(1+r_a\right)^y}\right) \tag{39}$$

where in the investment costs are included the cost of the conversion systems, the storage units and the pipes between different clusters (equation (40):)

$$CAPEX = \sum_{cs \in CS} (C^u_{cs} b_{cs} + C^v_{cs} P_{cs}) + \sum_{s \in S} (C^u_s b_s + C^v_s S_s + C^p_s P_s) + \sum_{p \in Paths} C^u_p d_p b_p$$

$$(40)$$

The costs for storage units and conversion systems are separated between a fixed cost per unit  $(C_{cs}^u \text{ and } C_s^u)$  and variable cost depending on the size of the unit  $(C_{cs}^v, C_s^v \text{ and } C_s^p)$ . Storage cost depends on the maximal capacity and on the compressor nominal power. The cost for a conversion system unit depends on the electrical nominal power. For the pipes, a nominal cost per distance  $C_p^u$  is assigned for each pipe p. This cost is assumed to be independent of the mass flow rate.

The operating costs include the cost of fresh material  $C_j^v$ , waste disposal  $C_i^v$ and electricity  $C_t^e$  (equation (41)):

$$OPEX = \sum_{t \in \mathcal{T}} \sum_{c \in \mathcal{C}, j \in J_v} C_j^v L_{c,j,t}^v$$

$$+ \sum_{t \in \mathcal{T}} \sum_{c \in \mathcal{C}, i \in I_v} C_i^v G_{c,i,t}^v + \sum_{t \in \mathcal{T}} C_t^e E P_t^{res}$$

$$(41)$$

# 4. Case study

# 4.1. Presentation

The model developed in section 3 is applied to the problem of designing <sup>420</sup> a hydrogen network, its supply via electrolyzers and hydrogen storage sizing. The territory is composed of three clusters associated with a hydrogen demand, distanced at 1 kilometre. A hydrogen network is introduced, with a linear cost of 500 $\in$ /m (Ghazouani, 2016). The objective of the case study is to demonstrate the relevance and pertinence of the model developed in this paper. Data

- <sup>425</sup> is inspired from Samsatli and Samsatli (2015). The cluster's hydrogen demand fluctuates between weekdays, weekend and seasons. Wind turbines are present in the cluster C1 and generates electricity, fluctuating between the seasons and during a day. In order to construct the time dependent dataset (hydrogen demand and electricity production), data from 8 typical days is used: 2 days
- (weekdays and weekend) for the four seasons winter, spring, summer and autumn. Each weekday is repeated 65 times and each week-end days is repeated 26 times. Each day is discretized into a period of one hour. In this way, the problem contains  $\mathcal{T} = 8736$  periods representing each hour of a year (52 weeks).
- An electrolyzer to be designed is placed in cluster C1. It will convert the available electricity in the territory into hydrogen, with a nominal ratio. The characteristics (ratio, cost) of the PEM electrolyzer are detailed in table 1. The water consumption for converting electricity in hydrogen is not taken into account here, assuming that water is always available, with a neglected cost and oxygen production is also not taken into account. We focus here on the hydrogen demand and the electricity consumption but the model could easily be extended, considering water and oxygen ratios, water availability and oxygen demand (which could provide income). The electrolyzer operating cost corresponds to the electricity consumption, when local electricity production is not
- <sup>445</sup> sufficient to cover the demand. Therefore, complementary electricity has to be imported from the grid. Electricity prices are detailed in figure 6.

#### Table 1

Characteristics of the conversion system PEM electrolyzer. Data from Samsatli and Samsatli (2015); Won et al. (2017); Jacobs (2016); Gorre et al. (2020) and own calculations

	Electric ratio $/H_2$ (kg/kWh)	CAPEX (fixed cost in $\in$ )	CAPEX (variable cost in $\in$ /kW)
Electrolyzer	$18.10^{-3}$	$3.10^{6}$	500



Fig. 6. Evolution of electricity prices for the 8 typical days, from Samsatli and Samsatli (2015).

The wind electric production is presented on figure 7. It varies hourly and seasonally. The hydrogen demand for the three clusters is presented in Figures 8

to 10. The demand is higher in summer and at 8am, 7pm and 10pm for the rest of the year. Figure 11 represents the difference between hydrogen production, assuming that all the electricity generated from wind turbines is used to produce hydrogen, with the conversion ratios presented in Table 1, and the demand for each hour of the year. The electricity production is not sufficient in summer during most part of the day, and at 7pm for a great part of the year.

In order to respond to the demand for these periods, two scenarios can be studied. Either electricity is imported and purchased from the grid, with an associated cost and is directly used to produce hydrogen. Or hydrogen is produced when there is a surplus of electricity (for example in winter) and is stored

<sup>460</sup> in a hydrogen tank. Then, stored hydrogen is delivered when there are electricity shortages, in summer or at 7pm for example. The optimization model can determine the balance between electricity imports or use of hydrogen storage, produced from local electricity.



Fig. 7. Electricity production for the 8 typical days, from Samsatli and Samsatli (2015)

The storage is placed in the cluster C1, close to the hydrogen and electricity production. Different cases are considered, in order to evaluate the pertinence of the compressed gas storage model:

• case (0): Without hydrogen storage

- case (1): An incompressible storage, without any compression costs.
- case (2): A compressible hydrogen storage, with compression energy costs.
- case (3): A compressible hydrogen storage, with compression energy costs and a compressor CAPEX.
- <sup>475</sup> The characteristics of the modelling cases are presented in table 2. For each storage model, different pressure discretizations are introduced, allowing a higher precision of mechanical work computation. The error committed due to the linearization will be estimated and compared in order to assess the pertinence of the discretization.
- For the compressed storage without any pressure discretization introduced, the electrical power for compression is 1.78 kWh/kg and it corresponds to an equivalent pressure of 77.8 bars (as if the gas was compressed at an equivalent pressure of 77.8 bars inside the storage). With one pressure introduced at 100 bars, the electrical power is 1.47kWh/kg (equivalent pressure at 39.3 bars) for
- $_{485}$   $\,$  the first interval and 2.09kWh/kg (equivalent pressure at 147.3 bars) for the

# Table 2

Characteristics of hydrogen storage

N' Case	Storage model	Pressure discretization	OPEX	CAPEX
1	Incompressible	-	-	500€/kg (Gorre et al., 2020)
2-a		1-200 bars	1.78  kWh/kg	
2-b	Compressible	1-100-200 bars	Depends on pressure state	500€/kg
2-c		1-66_33-200 bars	Depends on pressure state	
3-a		1-200 bars	1.78 kWh/kg	
3-b	Compressible	1-100-200 bars	Depends on pressure state	500€/kg + 2000€/kW (compressor) (Klumpp, 2015; Aarnes et al., 2018)
3-c		1-66-133-200 bars	Depends on pressure state	



Fig. 8. Hydrogen demand in the cluster C1 for the 8 typical days.

second interval. With two pressures introduced at 66 bars and 133 bars, the electrical power is 1.3kWh/kg (equivalent pressure at 26.5 bars), 1.9kWh/kg (equivalent pressure at 97.7 bars) and 2.15kWh/kg (equivalent pressure at 165 bars) for the first, second and third interval.



Fig. 9. Hydrogen demand in the cluster C2 for the 8 typical days.



Fig. 10. Hydrogen demand in the cluster C3 for the 8 typical days.



Fig. 11. Mismatch between hydrogen demand (aggregated) and instantaneous potential hydrogen production.



Fig. 12. Representation of the clusters C1, C2, C3 and of the potential hydrogen pathways. All clusters are 1km apart.

# 4.2. Design results

The case study is solved using CPLEX v12.7.1.0 solver (Nickel et al., 2021) on PC (Processor: Intelⓒ) Core™ i5-7200U CPU @ 2.50GHz - RAM: 16 Go -OS: Windows (C) 10). Table 3 presents the results: design of the electrolyzer, design of the hydrogen and CAPEX and OPEX for the different cases. The 495 benefit of a hydrogen storage is clearly shown. Without any storage, the electrolyzer must be sized in order to supply the demand, specially for the peak demand for summer at 7pm. In order to respond to the demand, the power of the electrolyzer is 47MW, 4 times bigger than the scenarios with hydrogen storage. Thus, even if there are no investments associated to storage, CAPEX 500 is higher. Moreover, as the electric production is not sufficient, electricity has to be bought from the grid, therefore OPEX is also higher. Including hydrogen storage reduces CAPEX and OPEX. It results in a smaller electrolyzer, around 12MW and independent of the hydrogen storage model. Indeed, hydrogen storage is used to shave the peak demand in hydrogen and avoid high electricity

<sup>505</sup> age is used to shave the peak demand in hydrogen and avoid high electricity prices. When storage is used, the share of renewable electricity rises from 69% to almost 89%. Moreover, the total cost (CAPEX + OPEX) is reduced by around 2.4 when storage is used. CAPEX is higher for case 3, but storage modelling includes compressor CAPEX which can explain that. OPEX is also higher for cases c because pressure discretization is finer. Thus, when hydrogen is stored

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at high pressure, compression cost is relatively higher for cases 2-c or 3-c than other cases (2-a, 3-a or 2-b and 3-b) with lower pressure discretization step.

Hydrogen storage behaviour depends on the daily demand for hydrogen and <sup>515</sup> renewable electricity production. The pressure inside the storage increases at the beginning of the day until 7pm, after which the storage is used to respond to the peak demand at 7pm (figure 13). Moreover, when electricity prices are high, for example at 5pm in spring, week-end, the electrolyzer is not running and hydrogen from storage is used to cover the needs. Conversely, the electrolyzer works at full power when electricity is available (self-consumption) or cheaper (in summer, weekdays after 10am). Actually, no electricity is bought during winter and autumn because local production is sufficient. Renewable electricity is used to satisfy the demand in winter and autumn but also to fill the storage, anticipating the periods when the wind is not sufficient or miss-

- ing. The hydrogen storage capacity is designed according to the peak demand in summer weekday and has a capacity of at least 2000 kg.(The difference between hydrogen demand and renewable hydrogen production is 2000 kg during a summer weekday (figure 11)). However, considering the day sequencing, the difference in a week is 3500 kg. Therefore, electricity still has to be bought from
- the grid because the storage capacity is not enough to cover the total demand throughout the year. Actually, hydrogen capacity design results in a trade-off between CAPEX and OPEX. The depreciation period in the case study is set at 5 years but extending it can lead to greater investments and lower OPEX. When a value of 20 years is used, the storage is two times bigger (4000 kg) and

 $_{\tt 535}$   $\,$  it results in a reduction of 38% of electricity bought from the grid.

For some cases ((2-c) and (3-c)), the optimality is not reached after 24 hours of computation. Indeed, these cases contain a lot of variables (binary and contin-

# Table 3

Design results for the different cases

Case	(0)	(1)	(2-a)	(2-b)	(2-c)	(3-a)	(3-b)	(3-c)
Electrolyzer power (kW)	46 954	12 020	$12\ 018$	12  019	12  019	12 018	$12\ 258$	$12 \ 019$
Flow max Electrolyzer (kg/h) $$	845	216	216	216	216	216	218	216
Volume Storage $(m^3)$	(-)	(-)	125	125	125	125	130	128
Capacity storage (kg)	(-)	2038	2053	2052	2053	2053	2132	2100
Compressor (kW)	(-)	(-)	386	453	465	385	387	409
Compressor consumption (MWh)	(-)	(-)	$909\ 237$	$881\ 201$	$826\ 071$	$1\ 077\ 838$	949  507	$866\ 203$
CAPEX (M $\in$ )	27.48	11.03	11.04	11.04	11.04	11.81	11.97	11.91
Total OPEX (M ${\ensuremath{\in}}$ )	4.43	1.56	1.58	1.58	1.62	1.58	1.54	1.60
$\mathrm{CAPEX} + \mathrm{OPEX} \ (\mathrm{M} \textcircled{\in})$	31.91	12.59	12.62	12.61	12.65	13.39	13.51	13.52
Tolerance	0%	0%	0%	0%	0.10%	0%	0.10%	0.10%
Share of renewable electricity	68.7%	88.7%	88.6%	88.6%	88.3%	88.7%	88.9%	88.4%

uous), making it difficult to solve them to optimality. Therefore, computational
difficulties are overcome by setting the design of the electrolyzer beforehand. Actually, the first results on cases 1, (2-a), (2-b) and (3-a) show that electrolyzer power does not depend on storage modelling and pressure discretization. Thus, the value of 12019kW obtained on cases 1, (2-a) and (3-a) is used on cases (2-c) and (3-c) to set the electrolyzer power and make the problem easier to solve.
The computation is stopped when the tolerance gap reaches 0.1%. Then, the

actual energy compression can be computed in post-processing and be used to evaluate the error due to the linearization in section 4.3.

# 4.3. Compression work precision

Because the compression costs are evaluated using a mean value for a certain <sup>550</sup> pressure interval, an approximation is realized. Actually, if the pressure interval is too wide, the mean value used for evaluating the compression cost can be far from the actual value. Particularly, when the storage is filled at low pressure, the compression work is over-estimated. In the opposite, when the storage is filled at high pressure, the compression work is under-estimated. Even if the cumulative error can balance itself through the time periods, the error is also re-

flected on the compressor design. Therefore, introducing intermediate pressure will reduce pressure interval sizes and reduce this approximation. Moreover, as





(c) Summer week



Fig. 13. Evolution of the pressure inside the storage for the first week of each season. The red dot lines correspond to the discrete pressures. Results for case (3-b)

we can see in figure 13, the pressure inside a storage can pass from one interval pressure to the next when filling (for example from 85 bars to 105 bars in a hour during a summer week). The computation of the mechanical work uses both mean values of mechanical compression (before filling and after) as shown in equation (26). This attempts to reduce the error.

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Results of compression work values are then compared to the exact values, without approximation. Storage pressure is computed from the ideal gas law (equation (19)), using the volume value and the hydrogen mass inside the storage obtained from the optimization. Then, mechanical compression work can be computed with the corresponding hydrogen flow at each hour without any approximation (equation (42)):

$$W_{electrolyzer,t}^{real} = L_t^{in} NCpT \left(\frac{P_t}{P_1}^{\frac{\gamma-1}{N\gamma}} - 1\right)$$
(42)

The actual design of the compressor can also be computed (equation (43)):

$$P_{electrolyzer}^{real} = \max_{t} \left( \frac{W_{electrolyzer,t}^{real}}{\delta_t} \right)$$
(43)

Results of the relative error due to the linearization are presented in table 4. The cases (0) and (1) are not included in the table because they do not include any hydrogen compressed storage model. The error committed on compression consumption decreases with the introduction of intermediate pressure, from 13%

- 575 to 10% concerning the total mechanical compression energy (for both cases (2-x) and (3-x)). The error on energy compression is relatively the same for the storage (2-a) and (2-b) (13% and a difference of nearly 114,000MWh) but the introduction of an intermediate pressure at 100 bars reduces the total energy consumption by 3%. Supposing an electricity price of 40€/MWh, it results in
- a cost savings of more than 1M€. (Note that in this case, local grid electricity is available from local production, that explains why there is no difference in OPEX in table 3 between case (2-a) and case (2-b), higher electricity consumption is absorbed by the local production). For compressor design, the error is

not relevant for cases (2-x) because compressor CAPEX is not considered, and has no influence on the optimization. For compression design, introducing a pressure discretization improves the precision, from 10% to 4% or 7% for the case 3.

Figure 14 compares the compression work obtained from optimization (xaxis) and with the value obtained from post-calculation (y-axis). The postcomputed value uses the exact pressure value inside the storage to compute the enthalpy compression, then the compression mass flow (get from optimization) is used to compute the energy compression. Three cases are presented on the figure: cases (2-a), (2-b) and (2-c). For instance for the case (2-b), one intermediate pressure is introduced (100 bars) and three discrete values are available

for enthalpy compression: one for a pressure state below 100 bars, one for a pressure state above 100 bars and one intermediate value (if the binary for pressure interval changes between two periods). These values are computed from equation (26) and are used in the optimization problem to compute compression
 work (x-axis).

The gap between the orange line 'y=x' and the blue crosses shows the precision on the compression work calculation. The error is lower as the blue cross gets closer to the orange line. If the blue cross is below the orange line, then the compression work is over-estimated. If the blue is above, the compression

work is under-estimated. This figure shows that the compression work is overestimated as the blue crosses are most-of-time below the line 'y=x'. Hence, the discrete value for enthalpy compression over-estimates its real value. Actually, increasing the number of discrete pressure (case 2-c) increases the precision on computation of the compression enthalpy and the blue crosses get closer to the

<sup>610</sup> line 'y=x'. The approximation of the pressure in the storage is better estimated, hence compression works also, particularly for high values of energy compression. Moreover, when the compression CAPEX is included (3-a, 3-b and 3-c), the error on compressor design decreases with the number of intermediate pressure. The error is only of 7% for the case (3-c) and 4% for the case (3-b). Using at least one intermediate discrete pressure seems to be enough to catch the actual size of the compressor and to provide a good estimation of the compressor consumption.

However, the tractability challenge must not be forgotten. If a great number
of discrete pressures are introduced, the number of variables rises sharply. For
each time period and pressure interval, two continuous variables and one binary
variable are defined for pressure characterization. Thus, at a constant number
of periods, the number of variables increases as the number of pressure steps are
specified. The problem could become quickly intractable in terms of solution
time or finding a solution. Therefore, a solution methodology must be established in order to compute complex case studies. The proposed methodology is

- The first step consists of solving the problem with a reduced number of pressure steps. Electrolyzers (or any conversion systems) are designed and an electric power is proposed. A certain volume of gas storage is also designed.
- 2. The second step uses results from step 1. Values of conversion system power and gas storage capacities are set, from step 1 results. It helps in reducing the size of the problem and a solution is found faster and easier.
- For example, for the cases 2-c and 3-c, without any predesign result, the optimality gap is stuck at about 30% after more than 24 hours of computing time. The duration is reduced to around 18,000 seconds (CPU time), showing the interest of the methodology.

# 5. Perspectives

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A comprehensive modelling structure for hydrogen generation, transport and storage optimization with a detailed model of compressed gas storage has been presented, but further improvements and works will be introduced to the model, based on this formulation:



Fig. 14. Comparison of the mechanical work obtained by the optimization (x-axis) versus the post-calculated value (y-axis)

#### Table 4

Error committed on mechanical compression and compressor design for the different storages

Case	(2-a)	(2-b)	(2-c)	(3-a)	(3-b)	(3-c)
Compressor (kW)	386	453	465	385	387	409
Compressor - real (kW)	411	405	406	422	371	379
Relative error (%)	6%	11%	13%	10%	4%	7%
Annual compressor consumption (MWh)	$909\ 237$	881 201	$826\ 071$	$1\ 077\ 838$	949  507	866 203
Annual compressor consumption - real (MWh)	795 526	$764\ 601$	743 $455$	$901\ 166$	$848\ 441$	$783\ 136$
Relative error (%)	13%	13%	10%	16%	11%	10%
CAPEX error (%)	0.00%	0.00%	0.00%	0.61%	-0.27%	-0.52%
OPEX error (%)	-0.38%	-0.14%	-0.07%	-0.38%	-0.25%	-0.08%

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- Part-load modelling. Actually, systems as electrolyzers or fuel cells do not operate at nominal performance 100% of the time. They can operate at part-load performance and see their efficiency be degraded or improved, compared to nominal performance. Hence, this aspect should be considered in multi-period problems, especially when intermittent energies are used.
- Tractability challenge. Computational issues can be observed because of the great number of continuous and binary variables and the considered time step here (1 hour). Increased time step durations could be studied, but this would impact the accuracy of intermittent electricity production data. A formulation in typical days could also be studied, but with particular attention on day sequencing in order to catch the storage dynamics through several days.
  - Energy (heat) and mass networks will be designed simultaneously. Indeed, the presence of conversion systems (such as electrolyzers) couples all the aspects of the problem. For a better comprehensive study of a territory, a systemic view of the problem will be carried out. It will lead to better solutions than treating each aspect (water, hydrogen, energy, heat, ...) separately.
  - Waste heat valorization at the compressor intercooler. In this way and

thanks to the new compressed gas storage model, compressor power can be estimated. Therefore, the compressor intercooling needs can also be estimated, and this waste heat could be recovered and valorized for thermal needs. This point is relevant to the previous one.

• An industrial park is a complex area of study. There can be competition in the use of resources, but also competition between industrial actors. Indeed, the model presented in this article assumes that each actor cooperates with each other and do not pay for the resource. It corresponds to a cooperative-game. However, in real life, industrials actors will seek its best economic interest, and will pay for the resource. As well, the distributor or producer will invest in the network and must be remunerated for the service. A competition appears between producer and industrial buyers appears. This will lead to non-cooperative scheme. Methodology will be investigated to model such kind of transaction.

#### 6. Conclusions and future work

- This paper presents a multi-period optimization linear model for the design of mass networks, including conversion systems and compressed gas storages. A generic model of conversion system is proposed based on its efficiency. A linear model of compressed gas storages is proposed based on pressure discretization, allowing the design of the compressor. The compressed costs can be computed and included into the objective function, the minimization of total costs (CAPEX + OPEX). The model is applied to a hydrogen case study
- inspired from the literature. The electricity generated from wind turbines is used to produce hydrogen to fulfill the hydrogen demands. Mass networks, electrolyzers and hydrogen (compressed) storages are designed. A comparison is done between results from optimization (linear model of compressed gas stor-
- <sup>690</sup> ages) and actual model of compressed gas storages. It shows that the electric consumption cannot be neglected in this case and the compressor power influences the solution. The approximation due to the linearization decreases as the

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pressure discretization is finer. However, the complexity of the model increases with the number of discrete pressures and the problem can become intractable,

- specially when a great number of periods or pressure steps are considered. A methodology based on pre-design is used in order to solve finer compressed gas storage model in an acceptable solution time. Numerous additions to the model have also been identified and can help us to increase the model reality: partload efficiency, coupling mass and energy networks, waste heat valorization at
- the compressor and modelling of competitive and individual interests of each actor and tractability challenge.

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system

# 705 Nomenclature

Subscripts and superscripts

	с	Cluster
	CS	Thermodynamic energy conversion
	i	Sink
710	j	Source
	m	Mass network
	р	Path
	r	Resource
	s	Storage
715	t	Time period
	v	Variable

Sets

$M_{net}$	Mass	networks
-----------	------	----------

- C Clusters
- 720 I Sources
  - J Sinks
  - P Paths
  - R Resources
  - S Storages
- 725 SC Conversion systems
  - T Time periods

#### Parameters

- $\delta_p$  Arbitrary direction of the path p
- $\gamma$  Constant heat capacity

# $_{730} \Omega$ Big number

- $\widetilde{w_{s,t}^{comp}}~$  Compression work of the gas storage s
- $\widetilde{w_{c,s,p}}$  Mean value of enthalpy compression in the pressure interval p
- $C_t^e$  Electricity price at time t
- $C_s^p$  Variable part for compressor cost
- $_{^{735}}\quad C^u_{cs}\qquad$  Fixed part for conversion system investment cost
  - $C_p^u$  Nominal cost per distance for a pipe
  - $C_s^u$  Fixed part for storage investment cost
  - $C_i^v$  Cost of material disposal in sink i

- $C_j^v$  Cost of material of source j
- $_{740}\quad C_{cs}^{v}\qquad$  Variable part for conversion system investment cost
  - $C_s^v$  Variable part for storage investment cost
  - $d_p$  Length of a pipe p
  - $EC_t$  Total electricity consumption at time t
  - $EP_{c,t}^c$  Electricity production inside a cluster c at time t
- 745  $EP_t^{limit}$  Limit of sold electricity to the grid at time t
  - $EP_t^{res,in}\,$  Electricity bought to the grid at time t

 $EP_t^{res,out}\,$  Electricity sold to the grid at time t

- $EP_t$  Total electricity production at time t
- $G_{c,i_r,t}$  Mass flow rate demand
- $_{750}~~L^{cs}_{c,j_f,t}~~{\rm variable\ mass}$  flow of the reference source  $j_f$  defining a conversion system cs at time t
  - $L_{c,j_r,t}$  Mass flow rate availability
  - $M_g$  Molar mass of the gas g
  - N Number of pressure stages
- $_{755}$   $N_y$  Number of operating years
  - $\begin{array}{ll} P^{cs}_{cs,t} & \mbox{Electrical consumption or production of the conversion system $cs$ at time $t$ } \\ & \mbox{t} \end{array}$
  - $P_{cs}^{cs}$  Electrical power of the conversion system cs
  - $P_s$  Compressor power of the storage s
- $_{760}$   $P_{s,i}$  Discrete pressure of the interval i

 $r_a$  Actualization ratio

 $rs_{j/i}$  conversion system efficiency associated to source/sink j/i

 $T_s$  Temperature inside the storage

 $V_{i_m,j_m}$  Volume of the gas storage  $(i_m,j_m)=s$ 

765 Continuous variables

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 $G_{c,i_r,t}^v$  Mass flow rate entering into a variable sink

 $L_{c,ij_r,t}^v$  Mass flow rate between a variable source and a sink

 $L_{c,i_r,t}^v$  Mass flow rate leaving a variable source

 $L_{c,s,t,p_s}^{p,in,after/before}\,$  Mass flow rate entering into the discretized gas storage at the pressure

 $L_{p,t}^{path}$  Mass flow rate through the path p

 $L_{c,ij_r,t}$  Mass flow rate between a source and a sink

 $Max\_S_{c,s_r}$  Maximum amount of resource r stored

 $Min\_S_{c,s_r}$  Minimum amount of resource r stored

775  $S_{c,s_r,t}$  Amount of resource r stored at time t

#### Integer variables

 $b^b_{cs}$  Binary indicating if a conversion system is used or not

 $b_{c,j_r,t}^{in}$  Binary indicating if the storage is filling

 $b_{c,i_r,t}^{out}$  Binary indicating if the storage is emptying

 $_{780}$   $b^P_{s,t,p}$  Binary indicating the pressure interval p inside the gas storage s

 $b_{c,s_r,t}^S$  Binary indicating if the storage is used

 $b_p$  Binary indicating if a path p is used

### Abreviations

CAPEX Capital expenditure

785 MILP Mixed-integer linear programming

**OPEX** Operating expenditure

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