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Identifying standard and simple designs of Power-to-Methanol processes: The costs of complexity reduction

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ABSTRACT

First industrial-scale Power-to-Methanol plants are starting to be deployed in various geographic locations to tackle the problem of high greenhouse gas emissions of the predominantly fossil-based production of methanol. With the aim to speed up the deployment by streamlining their engineering and construction, we explore the potential of reducing the complexity of designs to be distributed across locations with different renewable energy conditions. A multi-objective optimization-based method incorporating a broad process network for early-stage process synthesis is proposed, which by determining the installed capacities of technologies from the chemical production, utility and storage subsystems, identifies alternative designs with different levels of complexity along two dimensions: 1) the number of different technologies used, 2) standardization of designs across different locations. The method was applied to case studies, which paired together design locations with either wind- or solar-dominant renewable resource conditions in the US and Chile for standardization. As per the method, the increases of methanol production costs due to reduced design flexibility, inherently bound to complexity reduction, were quantified and Pareto fronts were constructed. These uncovered the possibility to significantly reduce the complexity of the designs with only small increases of the production costs. By comparing the results of the case studies under different cost and operation scenarios, we characterized general aspects, which need to be considered for such design simplification. One of the main outcomes were the quantified cost-increases due to standardization, which were around 7 and 15 % relative to the specifically designed plants for each location in the US and Chile case studies respectively. A subsequent analysis of the economies of numbers through learning rates reported in academic literature suggested that the proposed standardization, even across extremely different locations, could compensate these cost-increases and be economically beneficial. Yet, more specific data on achievable cost-reductions are needed, requiring more interaction with the industry and further research, for which we highlighted promising directions.

"*Perfection is achieved, not when there is nothing more to add, but when there is nothing left to take away.*"

Antoine de Saint-Exupéry

1. Introduction

Methanol is a crucial molecule for the chemical industry with an annual production capacity of 98 million tonnes (Mt), which contributes approximately 10% of the entire chemical sector's carbon dioxide emissions [1]. This supply primarily caters to the production of formaldehyde, acetic acid, and plastics, and if current trends persist, the demand for methanol could increase to 500 Mt per year by 2050 [2]. Beyond its crucial role as a bulk chemical, 31% of the produced methanol is used in fuel applications, including its direct use in automotive and marine transportation [1].

1.1. Why Power-to-Methanol?

To address the need to reduce greenhouse gas emissions associated with the conventional, predominantly fossil-based, methanol production, shifting to renewable sources of mass and energy is paramount. Such renewable methanol production currently only accounts for 0.2 Mt per year (mainly utilizing biomass as a feedstock), but various ongoing projects are expected to yield renewable methanol plants with

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a cumulative capacity of 8 Mt per year by 2027, with more than half to be produced in Power-to-Methanol processes [3]. These leverage renewable energy conversion (e.g. from solar and wind energy), carbon dioxide capture and water electrolysis technologies to supply the necessary mass and energy streams, without the limitations connected to biomass feedstock like resource availability, high land requirements or risks of biodiversity reduction [4,5], and therefore stand in the focus of this study.

1.2. Why distributed and standardized plants?

In order to mitigate global warming and its consequences a rapid reduction of green house gas emissions is required [6], making the fast deployment of such renewable technologies important. Additionally, recent military conflicts and supply chain disruptions have underscored the strategic value of reducing resource dependence on external suppliers and call for a swift deployment of renewable energy supply [7].

From the perspective of an engineering, procurement and construction (EPC) company, looking for solutions to satisfy the market demands for renewable methanol production amid these issues and to reduce the risk of highly capital-intensive investments, it is interesting to consider the potential of manufacturing higher number of standardized production systems distributed across various geographic locations, as opposed to larger centralized production plants.

Inspired by previous definitions reported within the manufacturing domain [8–10], one can define standardization in a general sense as an approach to reduce complexity [11], where the customization of products to exactly match market demands is deliberately limited, with the aim to increase the production efficiency and reliability through repetitive use of a common design features with the associated manufacturing, organizational and deployment procedures shared across several variants of the products.

Standardization and distributed production, closely linked to modular design principles, have already gathered attention in the process engineering community and were summarized in the work of Baldea et al. [12]. The authors provide an overview of the possible benefits offered by modularization, which can translate into significant cost savings and improved operation efficiency [12]. Under the concept of the economies of numbers (or learning-by-doing), the adoption of standardized modules facilitates manufacturing automation with reduced engineering and construction costs, shortened project timelines and lowered investment risks [12], which could address the uncertainties associated with an emerging market of renewable methanol production in politically and climatically turbulent times.

The summary of these qualitatively-stated benefits may seem promising, but without quantitative analysis would remain inconclusive. Addressing this are several modeling studies, which show the potential of the modular design concept in process engineering applications and are reported below.

By analyzing three distinct design problems using a generalized disjunctive programming approach for modular process design, Chen and Grossmann [13] demonstrate that modular design of distributed plants can be more economical than conventional centralized production in certain scenarios (yet with profit margins below 10%), warranting further investigation.

Bhosekar and Ierapetritou [14] propose a framework for comparing the supply chain for modular distributed plants and for a centralized plant and also consider the demand uncertainty [15]. Reducing the investment risk using modular technologies is investigated in stochastic programming formulation in [16]. Furthermore, a spatial superstructure generalization for the design of modular processes including the supply chain was developed by Shao et al. [17] who also identify modularity measures regarding connectivity, module size and transportation with an optimization approach for computing these [18].

The concept of unit design standardization across processes producing different products is explored in the work of Arora et al. [19] who show the potential benefits of reducing the capital intensity for small-scale production processes in this way on a case study including the methanol production process. Similarly, Stinchfield et al. [20,21] propose an optimization-based design approach for unit standardization across processes in the same family using surrogate models and demonstrate this for a water desalination and a carbon capture process.

Nonetheless, studies specifically focused on modular/standardized methanol production processes are scarce. Huang et al. [22] study the design, scheduling of a Power-to-Methanol where compression, synthesis and purification sections are considered as several standardized modular production lines, showing improved capability in dealing with fluctuating renewable resources due to the modular structure compared to a single (large-scale) production line. Yang and You [23] consider a modular methanol production facilities for utilization of shale gas in their techno-economic and environmental analysis, showing that the distributed modular design can outperform the conventional large scale production concept. Additionally, a couple of feasibility assessments of the Power-to-Methanol process at different plant sizes [24,25] have been reported, but no other works on modular production plants specific for methanol production could be found. For a comprehensive review of the Power-to-Methanol process please refer to [26]. In terms of other Power-to-X systems, Palys et al. [27] formulate an ammonia supply chain optimization model with modular power-to-ammonia processes, showing it can be more economical than conventional production and Sánchez et al. [28] investigate the associated scaling problems.

Though should distributed Power-to-X plants be specifically designed for locations with distinct renewable energy conditions or should we reduce the design complexity by standardizing across these locations? There is a lack of studies and design methods addressing such a standardization concept, which could support the development of distributed plants amid the aforementioned issues of slow deployment and resource autonomy. According to this standardization concept, an EPC company would offer a smaller number of standard plant designs and benefit from a more streamlined deployment process as opposed to designing a plant specifically for each location with a unique renewable energy resource profile to achieve a maximum efficiency at each location.

For Power-to-X processes, such a design should include the selection and sizing of technologies spanning the energy generation, utility, storage and chemical process subsystems, while considering the inherent fluctuations of the renewable resources at the different locations, which is a technological scope previously not considered in this context. We address this by proposing a design method, which can identify standard as well as specific designs from a broad process network including the dynamics of the renewable energy resources and allows for their economic comparison.

In the context of this study, a standard design is defined by a particular selection of major processing technologies and their capacities (i.e. sizes), as these determine, among others, the plant/module dimensions, arrangement and interconnections, which are crucial for designing the overall structure of the facility, organizing its production and planning its deployment. Such a standard design is then repeated in each installation of the production system, with the aim to achieve the aforementioned benefits in their manufacturing, construction and commissioning.

However, these benefits of design standardization are not readily quantifiable at an early stage of process development, due to: (1) the lack of detailed cost contribution data, where usually only total technology acquisition costs are known, (2) uncertain and often unavailable parameters describing the economy of numbers (learning rates) [29], (3) the requirement for models of limited complexity to keep the solution computationally tractable [30], especially if a large time-dimension is included.

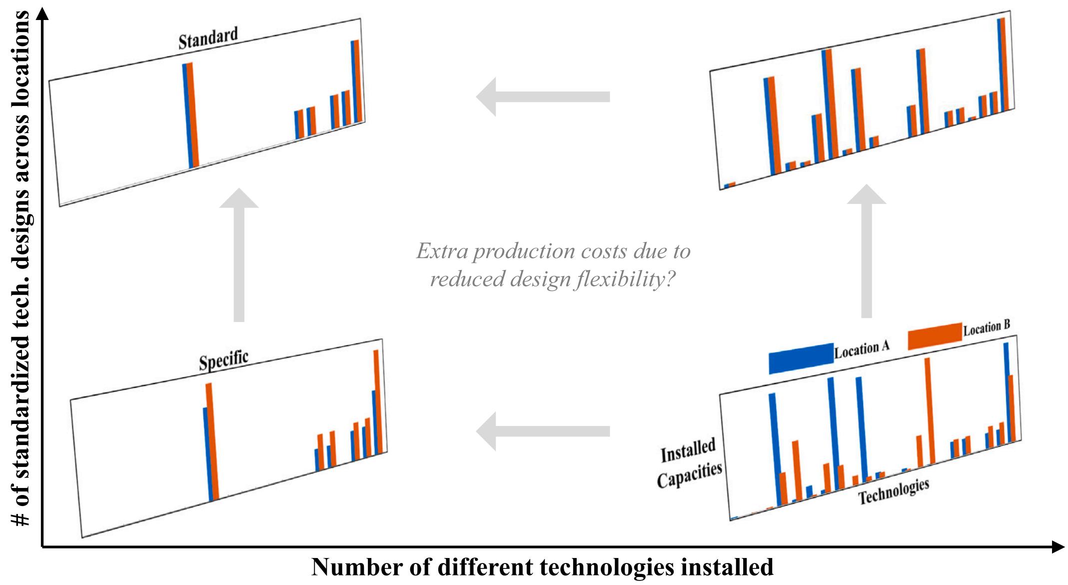


Fig. 1. Visualization of the concept of design complexity reduction studied in this work.

Hence, we instead quantify the cost-increases resulting from the degree of freedom/design space reduction due to standardization across the different deployment locations. This delivers a target for the required cost-reductions as a consequence of standardization, which need to be achieved to compensate the cost-increases relative to specific designs. This data should help the EPC company to make a better informed decision, if such a standardization concept should be investigated further, while considering the company-specific circumstances and experience. Additionally, as a further dimension of complexity reduction, we include a method to identify simple Power-to-Methanol plants to further reduce the design effort in deploying these "not perfect" but "good enough" designs.

1.3. Why simple plants?

Based on its translation from Latin, the term complex can be defined as consisting of many varied interrelated parts, while also interpreted as being complicated, involved or intricate [31]. It also implies a subjective difficulty in understanding or interacting with a system described as complex [31] and has been studied within the domains of biological, social, computer, management and engineering sciences [32].

Complexity of a chemical plant should not be understood purely in terms of its actual physical features (the product complexity), but rather of the whole development effort influencing the overall cost of the product, which is also affected by the market, organizational and process (designing, operating, manufacturing and deployment) complexities [32]. From this perspective, it is obvious that the development of a novel chemical plant, would indeed adhere to the definition of a complex system.

Yet complexity is an abstract concept, which is difficult to quantify with various measures and approaches being proposed [32]. A common sub-measure shared across a subset of the proposed methodologies is the number of components/elements/subsystems/technologies of the product [33–39]. Achieving simplicity along this measure (i.e. reducing the number of different technologies being installed, chosen for this exploratory study as a simple metric fitting to the early stage of process synthesis) holds a considerable appeal from the perspective of an EPC company, since it also directly ties to the aforementioned market, organizational and process complexities.

By opting for simpler plant designs in terms of the number of different technologies being installed, various benefits can be attained with a reduced equipment scope, such as a lowering the need for expert labor and decreasing the number of technology suppliers or necessary intellectual property acquisitions, leading to reduced administrative and legal burdens, which may be responsible for project delays. Moreover, simpler control schemes and maintenance procedures could make the plants more operationally manageable for the industrial practitioners.

However, such simpler designs are often left undiscovered by optimization-based design procedures, which opt to maximize the profit or minimize the production costs while disregarding the complexity tied to the resulting design [40], the consequences of which are not readily incorporated in a quantified manner into the optimization problem at an early stage of process synthesis, as mentioned in the previous section.

Thus, one of the goals of this study is to provide an approach, which would reveal these alternative designs and quantify the expected cost-increases due to the limitation of the degrees of freedom when forcing a simple design. This should help in removing the unnecessary complexity of the designs and allow the experts to identify potential design candidates to be investigated further in more detail. Additionally, this is to be done in parallel with the aforementioned standardization of designs across locations, to see if these two forms of complexity reduction influence each other.

Consequently, in the following sections of this article we propose a method to calculate the extra production costs associated with the complexity reduction due to standardization across locations and limitation of the number of technologies being installed (Fig. 1). Furthermore, by applying the method on two case studies of Power-to-Methanol plant design in the US and Chile under different cost and operation scenarios, we provide an overview of alternative designs of different complexity to support the decision making of engineering companies and identify important aspects, which should be considered for such complexity reduction. Finally, we quantify the required learning rates needed to compensate for the decreased design flexibility and compare them to learning rates reported in scientific literature, showing the potential of the proposed complexity reduction.

2. Methods

The methods section is structured as follows: First, the used modeling method together with extensions needed to identify simple and

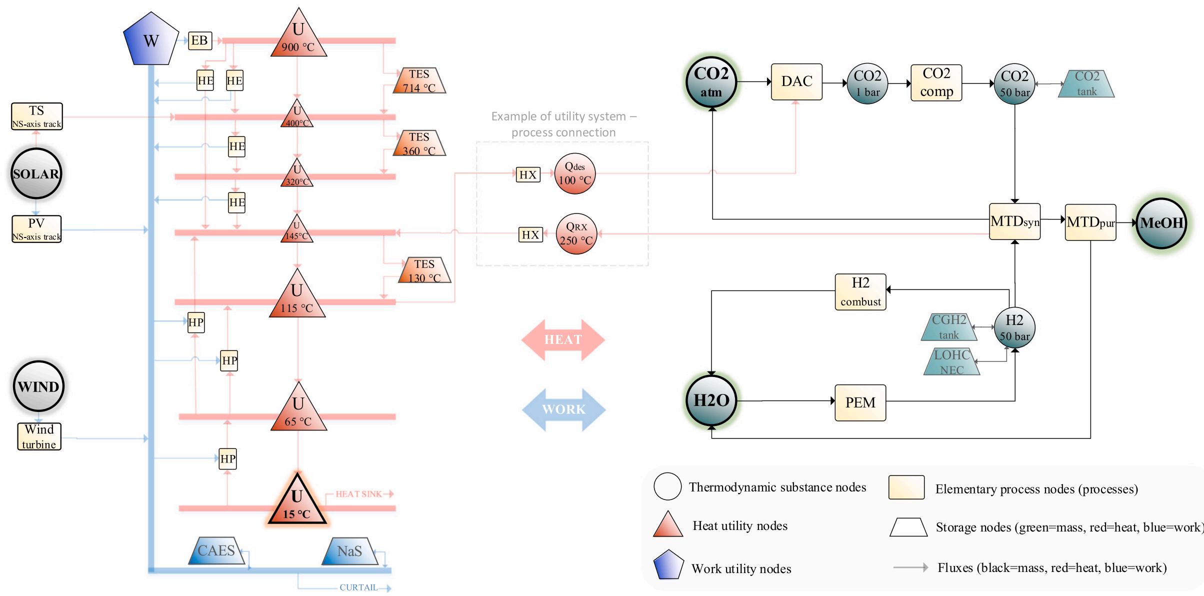


Fig. 2. Process network considered for the Power-to-Methanol designs.

standard designs are explained. Afterwards, the selection of considered sub-processes of the Power-to-Methanol and the locations is reasoned. Furthermore, the renewable resource data, the plant capacity and the cost/operational scenarios used are reported. Finally, the implementation and solution of the model are commented on.

2.1. Underlying modeling method

At an early stage of process synthesis, considering a broad scope of technologies can lead to the identification of interesting design solutions. Yet this is complicated for processes supplied by renewable energy sources fluctuating on an hourly, daily and yearly basis, as dynamic operation with an extensive time-domain needs to be taken into account, which substantially increases the computational complexity. To address this, the mathematical complexity of the models needs to be limited to make the design problems computationally tractable [30]. This applies also to this work, where modeling of the Power-to-Methanol process is done according to the FluxMax approach.

2.1.1. FluxMax approach

The FluxMax approach is an optimization-based design method, which by discretization of the thermodynamic state space (in this work, the temperature levels of the utility subsystem Fig. 2) decouples nonlinearities from the optimization problem leading to a linear network flow optimization problem. By the inclusion of an heat integration model, the method allows to consider the design, scheduling and waste-heat utilization (either through heat integration or technologies like heat pumps or heat engines) in parallel. In order to properly model the storage processes and the energy generation technologies a time-domain is included and discretized with a resolution of 1 h, spanning one representative design year, which was time-aggregated to reduce the overall model complexity (more details in Section 2.4). Operation constraints, like ramping limits and minimum production capacities are also included. A detailed description of this method can be found in [40] and its further use for multi-objective optimization of renewable methanol production through the biogas and Power-to-Methanol process routes in [41]. Hence, in the main body of this article we include only the fundamental equations of mass and energy balances and operation constraints for a fast overview. The full optimization problem can be found in section S8 of the supplementary material.

The processes of the process network are modeled using the process extent variables λ together with the generalized stoichiometric coefficients χ and are used to calculate the internal fluxes of heat, mass or work according to:

$$F_{(loc,c_{nonstor},p,t_k,t_g)} = \lambda_{(loc,p,t_k,t_g)} \chi_{(c_{nonstor},p)} \tag{1}$$

The external fluxes entering or leaving the process network are calculated by:

$$F_{ext(loc,c_{nonstor},tk,tg)} = \sum_p \lambda_{(loc,p,tk,tg)} \chi_{(c_{nonstor},p)} \tag{2}$$

The process extent of a process p in location loc in a typical day t_k and an hour t_g is limited by the nominal process extent λ_{nom}, which determines the installed nominal production capacity of the process in a location:

$$\lambda_{(loc,p,t_k,t_g)} \leq \lambda_{nom(loc,p)} \tag{3}$$

The mass/energy balances of the storage processes used to determine the stored amount $S_{(loc,c_{stor},t_i,t_g)}$ and its change during time increment dt, which also model the self-discharging of storages as determined by the self-discharge coefficient $\kappa_{(c_{stor})}$, are described according to:

$$S_{(loc,c_{stor},t_i,t_{g+1})} = S_{(loc,c_{stor},t_i,t_g)} + dt \left(\sum_p \lambda_{(loc,p,t_k,t_g)} \chi_{(c_{stor},p)} - \kappa_{(c_{stor})} S_{(loc,c_{stor},t_i,t_g)} \right) \tag{4}$$

The storage amount is limited by the installed nominal storage capacity:

$$S_{(loc,c_{stor},t_i,t_g)} \leq S_{nom(loc,c_{stor})} \tag{5}$$

The operation constraints are composed of the ramping limits:

$$\frac{\lambda_{(loc,p,t_k,t_{g+1})} - \lambda_{(loc,p,t_k,t_g)}}{dt} \geq -1(ramp_{limit(p)} \lambda_{nom(p)}) \tag{6}$$

$$\frac{\lambda_{(loc,p,t_k,t_{g+1})} - \lambda_{(loc,p,t_k,t_g)}}{dt} \leq ramp_{limit(p)} \lambda_{nom(p)} \tag{7}$$

and the minimum production capacity limits:

$$\lambda_{(loc,p,t_k,t_g)} \geq \lambda_{nom(loc,p)} minCAP_{(p)} \tag{8}$$

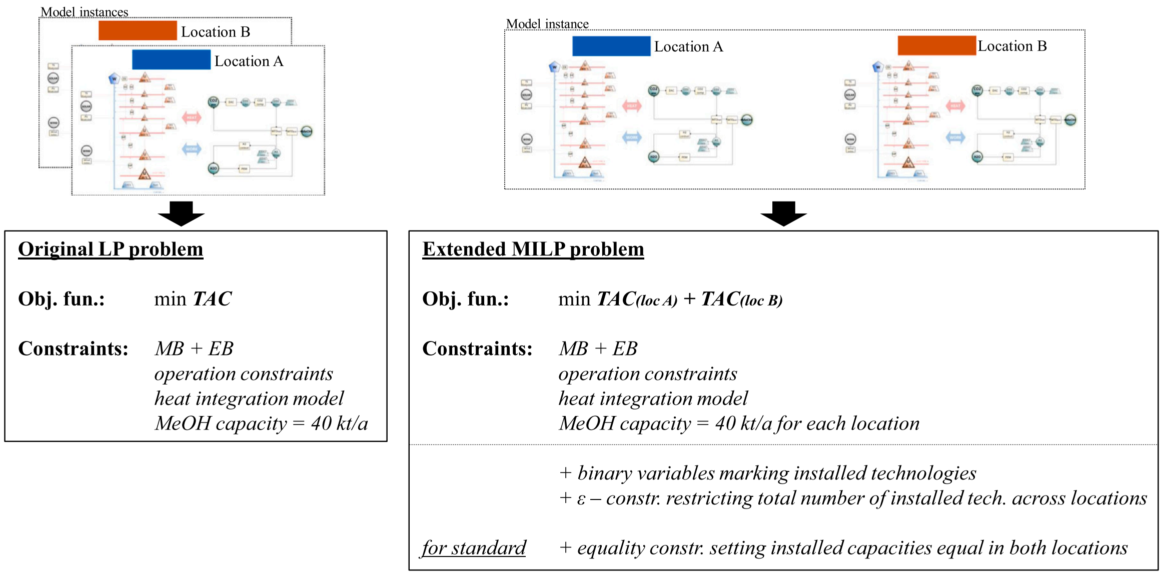


Fig. 3. Visualization of the adjusted optimization problem for the identification of simple designs standardized across locations exemplified on a two location problem.

The parameter values of these limits are shown in section S5 of the supplementary material.

As seen in Fig. 2 there are many production pathway alternatives to select from among the different utility, storage and energy generation processes depending on the renewable energy conditions in a particular location. In the next subsection we describe the model extensions to identify and compare these design alternatives according to their complexity through multi-objective optimization, while also considering design standardization across different locations.

2.1.2. Model extensions to identify simple and standard designs

The extensions to the original linear programming (LP) problem, which solves only one model instance (with renewable resource data from one location) at once, are visualized in Fig. 3. In order to identify the extra costs due to standardization, the model is extended to include the design for multiple locations in parallel. As a consequence the economic objective function of total annualized Capex (TAC), into which we also include the operation and maintenance costs and indirect Capex investment, commonly estimated as a percentage of the processing equipment Capex [42], is composed of contributions from each location considered:

$$\sum_{loc} TAC_{(loc)} = \sum_{loc} CAPEX_{total(loc)} f_{cr} (1 + f_{O\&M} + f_{indirectCAPEX}) \tag{9}$$

with the capital recovery factor f_{cr} being equal to:

$$f_{cr} = \frac{i(i+1)^n}{(i+1)^n - 1} \tag{10}$$

taking the lifetime n to be equal to 25 years and an interest rate i of 7% was assumed similarly as in comparable studies [43–45]. The operation and maintenance cost factor $f_{O\&M}$ was taken as 4% of the total Capex and the indirect Capex costs were estimated to be 11% based on standard costing methods [42].

This objective function was chosen because the vast majority of Power-to-Methanol production costs are required for the investment into and the operation of technological assets [43,44,46] since there are essentially no feedstock costs for air and salt water (more details on location selection in Section 2.3). Labor costs were excluded, as they were shown to be relatively small [40,43] and would be identical for each location as calculated based on the simple estimate model used for early stage process design [42] (see also section S2 in the supplementary material). Furthermore, as we analyze the results from a learning rate perspective (Section 3.6), excluding cost factors not directly related to the Capex is needed as learning rates only refer to Capex reductions [29]. This is also the reason why the levelized costs of methanol are not reported in this study. In the result figures, we rather relate the total annualized Capex to the yearly methanol production capacity, which are nevertheless comparable to the levelized costs reported in similar studies [40,43,45], since the labor costs are relatively small.

Going further into the terms of the objective function, the $CAPEX_{total(loc)}$ is the sum of all acquisition costs (including engineering, construction and material costs) of the energy generation technologies, processes (utility and chemical) and storages:

$$CAPEX_{total(loc)} = \sum_{gen} inst_{g(loc,gen)} CAPEX_{(gen)} + \sum_{p} \lambda_{nom(loc,p)} CAPEX_{(p)} + \sum_{c_{stor}} S_{nom(loc,c_{stor})} CAPEX_{(c_{stor})} \tag{11}$$

where $inst_{g(loc,gen)}$ is the nominal installed capacity of the generation processes. All acquisition cost parameters for energy generation technologies ($CAPEX_{(gen)}$), processes ($CAPEX_{(p)}$) and for storages ($CAPEX_{(s)}$) are summarized in sections S5 and S6 of the supplementary material respectively.

The total number of installed technologies is used as a simple measure of design complexity in this study (reasons commented on in Section 1.3). In the context of this study, we define a technology as a standalone functional element of the highest level within the process network (e.g. meaning that a process unit like water purification needed upstream the water electrolyzer is a sub-unit of the overall PEM electrolyzer technology and not considered as a separate technology). Furthermore, the technology is characterized by having a technology provider (be it an external or an internal supplier within the EPC company considered in this study) who is responsible for its function described by defined input and output streams with a dedicated control scheme allowing for independent operation, making it usable as a part of different processes (e.g. the PEM electrolyzer process could also be used in other Power-to-X processes).

Naturally, selection of the particular technologies according to this definition can be subject to interpretation, is dependent on the actual product definition of the suppliers and hence is subject to expert judgment based on the experience within a particular company applying this method. Based on independent costs for individual technologies reported in literature, we assign the technology tag to the major processes within the process network (all of the storage processes, the electric boiler, heat engines and heat pumps of the utility processes, the energy generation processes and to processes of the chemical process subsystem).

In order to limit the complexity of the design in terms of the number of installed technologies, binary variables xg, xp and xs are introduced, which mark the installed technologies and serve to calculate the second objective function of the total number of selected technologies across locations N_{tech} according to:

$$N_{tech} = \sum_{gen} xg_{(gen)} + \sum_{p_{integer}} xp_{(p_{integer})} + \sum_{c_{stor}} xs_{(c_{stor})} \tag{12}$$

where the $p_{integer}$ subset marks the processes, which are optional and subject to selection as opposed to those processes, which need to always be selected in the process network (methanol synthesis process, the water electrolyzer and a direct air capture process with CO_2 compression).

The second objective function (N_{tech}) is included into the optimization problem according to the ϵ-constraint method and the total number of allowed installed technologies (ϵ_{limit}) is consecutively reduced, to produce the desired Pareto fronts describing the trade-off between the TAC and the number of utilized technologies:

$$N_{tech} \leq \epsilon_{limit} \tag{13}$$

To identify standardized designs across the different locations, there are two model settings defined. The first allows the designs to be specific for each locations (installed production capacities of the individual technologies in the different locations are independent from each other). The second, forces the installed capacities to be equal in all of the different locations, forcing the designs to be identical across the different locations (exemplified on a pair of locations A and B):

$$\lambda_{nom(\mathtt{loc\ A},p_{common})} = \lambda_{nom(\mathtt{loc\ B},p_{common})} \tag{14}$$

$$S_{nom(\mathtt{loc\ A},c_{stor})} = S_{nom(\mathtt{loc\ B},c_{stor})} \tag{15}$$

The exception are the energy generation technologies (PV panels, parabolic troughs and wind turbines) for which the installed capacity should be adjusted for each location (otherwise standardizing across solar-dominant and wind-dominant locations would lead to extremely costly and consequently noncompetitive designs).

2.2. Process selection

The selection of the processes to include into the overall process network (Fig. 2) was supported by the results from our previous work [40], which included a larger process network and the most promising technologies identified were selected into the process network in this work. The reason why such a larger process network was not included in this work was the significant increase in computational effort required to solve the system for (in the presented cases) for two locations at once. The parameter values for the generalized stoichiometric coefficients χ describing the material and energy streams of the processes are reported in section S7 of the supplementary material.

2.2.1. Energy generation subsystem

For the energy generation subsystem three different technologies were selected: the wind turbine, north-south oriented horizontal axis tracking photovoltaic (PV) panels and parabolic troughs (TS), which concentrate solar irradiation to heat up an energy carrier and capture thermal solar energy at 400 °C [47]. This thermal solar technology was selected also due to their modular structure deployable at a smaller-scale installations investigated in this study.

The model of the wind turbines was selected to be the 3.0 MW Vestas V90 turbine with a performance curve described by a cut-in speed of 4 m/s, minimum speed at top capacity of 15 m/s and a cut-out speed of 30 m/s [48]. The solar generation technologies are characterized by their efficiencies of converting solar irradiation hitting the aperture area (calculation described in section S3 of the supplementary material) into a useful form of energy. For the PV panels generating electricity an average efficiency of 15% is assumed [49] and for the parabolic troughs a thermal efficiency of 65% for systems delivering 400 °C heat [47].

2.2.2. Chemical process subsystem

Given our focus on the potential application of harnessing off-grid renewable resources in a smaller-scale methanol plant, our investigation focuses on the direct methanol synthesis pathway. This choice is motivated by its relative simplicity compared to the CO-based process, as it eliminates the need for a reverse water gas shift reactor and leads to reduced by-product generation resulting in a simpler purification section [50]. Notably, a long-running 4000 tons per year industrial plant underscores the viability of this direct methanol production pathway [50]. We omit the electrochemical methanol production from the process network due to its currently prohibitive cost and excessive energy consumption [51]. The direct methanol synthesis process (MTDsyn) and the purification process (MTDpur) were modeled in Aspen Plus to calculate the mass/energy streams and are described in detail in section S1 of the supplementary material.

A range of options exists for the direct air capture process (DAC), each offering distinct advantages. The high temperature adsorbent DAC approach, employing a CaO-based hydrogenation and dehydrogenation cycle, is particularly well-suited to larger scale applications where economies of scale mitigate the impact of higher initial investments [52]. Conversely, the liquid absorbent method proves less optimal for DAC due to the substantial air volumes necessitating processing. Addressing the challenge of solvent evaporation incurred by this approach comes at a considerable expense [53]. Among the available low temperature DAC techniques utilizing modular adsorbent designs, we have opted for the established Climeworks process [54], which demands an electricity input of 400 kWh/t_{CO_2} and consumes 2000 kWh/t_{CO_2} of desorption heat at 100 °C [55], which is suitable as a heat sink for the waste-heat generated in the methanol synthesis process for example. The CO_2 compressor (CO2comp) was modeled in Aspen Plus as a 5 stage multi-stage compressor with inter-stage cooling (section S1 of the supplementary material).

The polymer-exchange membrane water electrolyzer (PEM) was selected as a technology with a high technology readiness level (TRL) compared to the solid-oxide water electrolyzer and a better dynamic characteristics than the alkaline water electrolyzer for direct connection to renewable resources [56]. The PEM process delivers compressed hydrogen at 50 bar and operates at a temperature of 80 °C [56] and also incorporates a hydrogen purification process (temperature-swing adsorption). The detailed modeling of the PEM process is described in section S1 of the supplementary material.

As we focus on coastal locations in the presented case studies, desalination of water would be a process, which would be included into the design, to supply the necessary process water. However, in order to limit the complexity of the model, we do not include desalination technologies into the process network, due to the fact that they have very little impact on the overall design and costs as our previous study has shown [40].

Among technologies, which can reconvert energy vectors (H_2 in our case) back to electricity/high temperature heat, we include only the combustion of H_2 (H2comb), modeled based on the lower heating value of H_2 and efficiency of 92%, since the PEM fuel cell was never selected in our previous study [40]. On the other hand, methanol converting processes (methanol combustion, methanol fuel cell) would consume the only product desired in the studied designs, so it would make little sense to reconvert it back to energy.

2.2.3. Utility subsystem

Since according to the FluxMax approach the utility subsystem is modeled by the discretization of the thermodynamic state space, the concrete heat utility nodes (HUNs) representing the utilities supplying/extracting heat (i.e. steam at a particular pressure level) need to be chosen before solving the optimization problem. These are connected by utility processes of heat exchange (HX), cooling (CL), heat pumping (HP) and heat engines (HE) (Fig. 2), which facilitate energy exchange between them.

The selection of the temperatures at which these HUNs operate was done according to the temperatures of streams in the chemical and energy generation subsystems. As the highest temperature inside the system we take 900 °C to model the potential to generate high temperature heat through combustion and electric heating (EB). HUN at 400 °C was selected as thermal solar energy generation technology (parabolic troughs) serves as an important alternative to supply the system with high-temperature heat at this temperature. Discretization has been selected to be more dense between 400 °C and 65 °C because this is where the most waste-heat utilization potential can be materialized with the majority of heat streams being in this interval.

Based on the selected temperatures of the HUNs, the connectivity of the utility processes and the heat streams of the chemical and energy generation subsystems can be determined. This is done following physico-technical rules, which make sure that energy balances and the second law of thermodynamics are obeyed and a sufficient temperature difference between heat transferring streams is maintained (10 °C). The details of these connectivity rules are explained in [40] with the overall results for this process network (the generalized stoichiometric coefficients) are reported in section S7 of the supplementary material.

In accordance with established practice [40], the generalized stoichiometric coefficient of the high-temperature heat flux in a particular process is assigned a value of 1 (when it functions as a heat sink) or −1 (when it serves as a heat source) the coefficients of other heat streams are calculated based on efficiencies. For the heat pumps, the generalized stoichiometric coefficients is derived from the coefficient of performance (COP), with the second law efficiency $\eta_{2\text{nd}\ law}$ set at 40% as per the work by Stampfli et al. [57].

$$COP_{HP} = \frac{T_{hot}}{T_{hot} - T_{cold}} \eta_{2\text{nd}\ law} \tag{16}$$

Furthermore, a restriction was enforced on the maximum temperature lift, capping it at 80 °C, and the upper boundary for the heat sink temperature is currently constrained to 160 °C, due to the prevailing technological capabilities, as noted in the study by Wolf et al. [58].

Regarding the heat engine (HE) processes, which, for the purposes of this study, exclusively encompass steam turbines (since organic Rankine cycles, with relatively high cost parameters were not a significant pars of the designs in our previous study [40]) are modeled according to the overall efficiency, which is determined from the Carnot efficiency and the second law efficiency of 50% [59]:

$$\eta_{HE} = \frac{T_{hot} - T_{cold}}{T_{hot}} \eta_{2\text{nd}\ law} \tag{17}$$

Additionally, a 60 °C minimum temperature difference between the heat source and heat sink is enforced with a 120 °C limit for the lowest heat sink temperature for a steam turbine.

In the case of the electric heating/boiling process (EB), the generalized stoichiometric coefficients are derived from the efficiency associated with the conversion of electricity into heat, denoted as η_{EB} and specified as 92%. Please note, that additional removal of utility processes, which were in accordance to the aforementioned physico-technical rules has been carried out, where similar HPs and HEs have been excluded to limit the complexity of the model, in order to include just distinct pathways for supplying the energy to the Power-to-Methanol production system.

Table 1
Parameters of energy (work) storage processes (adiabatic compressed air energy storage: CAES and NaS molten salt battery: NAS), where applicable converted to $ from EUR with a conversion rate of 1.18 $/EUR.

	CAES	NAS	Ref.
Storage section costs ($/kWh)	129	352	[62]
Conversion system costs ($/kW)	998	432	[62]
Round-trip efficiency (%)	65	83	[62,63]
Self-discharge rate (%/d)	0	20	[62]

Table 2
Selected latent heat energy storage.

Phase change material (PCM)	T_{melt} (°C)	Latent heat (kJ/kg)	Density (kg/m^3)	PCM cost[a] ($/kg)	Ref.
$MgCl_2$	714	452	2320	0.35	[64,65]
NaCl–KCl (58:42)[b]	360	119	2085	0.14	[65]
HDPE[c]	130	255	952	0.49	[66]

[a] Recalculated with exchange rate of $/EUR = 1.18 and EUR/GBP = 1.17.
[b] Mass ratio.
[c] High density polyethylene.

2.2.4. Storage subsystem

Intermediate storages of mass, work and heat were included to allow for decoupled dynamic operation of the processes from the fluctuations of the renewable energy resources. The most promising mass storages among the alternatives in our previous study were identified to be the CO_2 storage, compressed hydrogen storage and hydrogen storage in liquefied organic hydrogen carrier (LOHC) [40].

The CO_2 is stored as a liquid at 71 bar and 30 °C with an extra compressor stage with cooling used as the charging process [60]. The hydrogen is compressed up to 200 bar to be stored in the CGH2 process with a compression energy demand of 1.1 kWh/kg [61]. The LOHC storage uses N-ethyl-carbazone (NEC) to store hydrogen bound in a liquid form using a cycle of hydrogenation (charging) and dehydrogenation (discharging), which introduces the potential of utilizing waste-heat in these conversion processes. Detailed data describing the LOHC system can be found in [40].

Upon review of the results of this study, one interesting hydrogen storage alternative, which we have not considered in the process network warrants mentioning for future consideration. It is using methanol as a hydrogen carrier itself and utilizing the methanol synthesis reactor as the hydrogenation process, saving one processing step compared to the considered LOHC alternative. Yet, this would be at the cost that the dehydrogenated form of methanol would be a gas at ambient conditions (CO_2) with consequences for the storage Capex and energy requirements, which would need to be evaluated.

The process network incorporates two distinct options for energy storage in the form of electricity: above-ground adiabatic compressed air energy storage (CAES) and NaS molten salt batteries (NAS), which were predominantly modeled using data compiled from the research conducted by Zakeri et al. [62] and their characteristics are summarized in Table 1.

The selection of thermal energy storages (TES) was carried out from the phase change materials (PCM) gathered in several reviews [64–66]. The ones with a fitting melting temperature were selected to provide a high, medium and low temperature options of heat storage for the utility system. The characteristics of the selected PCMs are summarized in Table 2. Across all the chosen TES, a heat loss of 5% from the stored heat and a self-discharge rate of 0.5% per day are applied [67]. An overview of storage parameters can be found in section S6 of the supplementary materials.

2.3. Location selection

There were two criteria when selecting the locations for the case studies considered within this work: (1) they should be coastal locations

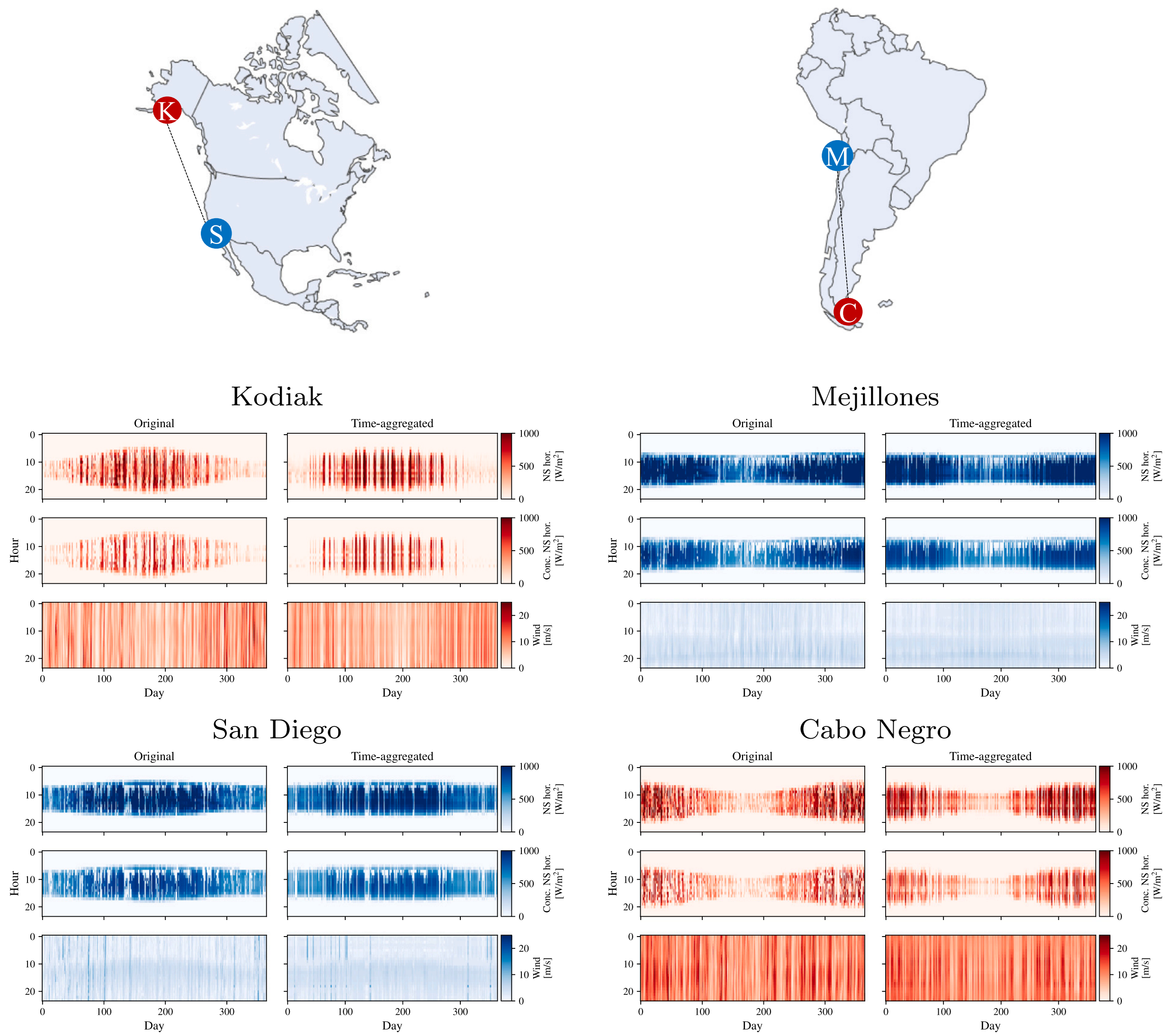


Fig. 4. Location pairs considered for the standardized design of Power-to-Methanol plants including the renewable resource data (solar irradiation hitting the aperture area for a north-south (NS) horizontal axis tracking PV panel and concentrating parabolic trough) in its original and time-aggregated form using 10 typical days.

with access to sea water to prevent putting extra pressure on locations with limited water supply as well as the possibility to ship the methanol or directly use it as a fuel in the shipping industry, while also allowing the transport of plant components during construction, (2) since one of the goals of this study is to determine the extra costs due to inter-location standardization, locations were paired in such a way as to combine extremely opposite renewable energy profiles (solar and wind dominant), representing a worst-case scenarios, which poses the largest challenge to standardization and hence the highest cost-increases due to a loss of degrees of freedom.

The resulting location selection with their renewable profiles can be seen in Fig. 4. As the first pair of locations for the design we have a wind-dominant location of Kodiak in Alaska (latitude: 57.79, longitude 152.43), where a wind-turbine park is already located. As the solar-dominant location in this pair, we take the San Diego in California (latitude: 32.61, longitude −117.10) on the coast near an industrial site.

For the second pair we select two outstanding locations regarding renewable resources in Chile. The solar-dominant location can be found in Mejillones (latitude: −23.08, longitude: −70.38) where there is already a chemical production park including shipping terminals. Cabo Negro in the south of Chile (latitude: −52.94, longitude: −70.81) directly next to an already existing methanol production plant with the associated infrastructure.

2.4. Renewable resource data

Data pertaining to solar energy renewable resources was sourced from the National Solar Radiation Database of NREL [68]. In this context, the typical meteorological year (TMY) data with a 1-h resolution was employed, which stands for a median meteorological year established within the time-frame from 1998 to 2019 [69]. The dataset encompasses parameters such as global horizontal irradiation (GHI), direct normal irradiation (DNI), diffuse horizontal irradiation (DHI), surface reflectivity ρ, and solar zenith angles θ_Z. These constitute the input for solar irradiation models, which compute the total irradiance striking the aperture area of solar generation technologies, accounting for their spatial orientation in relation to the sun's position (section S3 in the supplementary materials).

Wind speed data (1 year with a resolution of one hour) has been gathered from Renewables.Ninja [70,71] where one can access the MERRA-2 meteorological model retrospective global predictions [72] for the year 2019, which was chosen as the design year for the study, as no freely accessible TMY data for the wind speed profiles is available. Please note that there is one exception and that is for the wind speed data for San Diego, which have been gathered from the Wind Toolkit from NREL [73] using the Wind Prospector tool for the latest available year of 2012 (WindToolkit side ID: 287988), unfortunately, the tool has been discontinued during the preparation of this study [74]. However, since the wind speeds are low in this location and, as also predicted by MERRA-2, would even be below the 4 m/s minimum wind turbine wind speed, we keep the original data from WindToolkit since it does not affect the selected designs.

Subsequently, the renewable resource profiles underwent aggregation into typical days, a process facilitated by the application of the k-medoid clustering algorithm using the *tsam* framework [75]. Prior investigations by the creators of *tsam* have elucidated the implications of time-series aggregation, as well as the ramifications of the number of chosen typical days. Within the context of a fully renewable-centered energy system featuring seasonal storage, the precision of the identified system configuration remained relatively unaltered beyond the threshold of 12 typical days. Notably, the associated inaccuracies in annual cost estimations remained below 5% [76].

In this work a more aggressive time aggregation was required as design problems in two locations needed to be solved simultaneously and multiple times to construct the Pareto fronts. Therefore, 10 typical days were chosen as an acceptable trade-off for the given computational resources (aggregated profiles shown in Fig. 4), which is supported by a sensitivity analysis to the number of typical days presented in section S4 of the supplementary materials.

2.5. Plant capacity

An important part of the design is setting the desired production capacity for the Power-to-Methanol plants. Here we have oriented ourselves on the current market of industrial scale renewable methanol demonstration plants that are starting to appear and are offered by design and EPC companies.

An overview of the planned projects can be found in [3], where plants were announced with a capacity ranging from 50 000 to 250 000 t/y of methanol. However, for the distributed production concept targeted in this study a smaller production plant capacity of 40 000 t/y has been chosen, based on the skid-mounted methanol production modules for decentralized production offered by [77] and the upper capacity of 100 t/d for renewable methanol plants offered by [78]. An example of a plant of a similar capacity (32 000 t/y) is already under construction in Denmark [79].

Putting the chosen plant capacity into perspective, to cover the total methanol production in the US in 2018 of 5.7 million metric tons [80] (ca. 5% of the global production capacity) there would be 144 of these plants needed. Naturally, it is not expected that the whole methanol production would be covered by just this one design concept, but a certain market-share, especially in remote locations for autonomous production could be covered with such standardized stand-alone designs benefiting from the economies of numbers.

2.6. Scenario definition

To construct the four different scenarios studied in this work, two different aspects of the production were varied: (1) costs and their expected development in the next years and (2) the operation flexibility of the methanol synthesis.

2.6.1. Cost scenarios

Two different sets of technological cost scenarios were considered. The first one covers costs, which were gathered from open literature reported for the costs up until the year 2018 representing the current situation (baring in mind a certain delay of reporting of current costs appearing in the literature and the consideration of a large process network of non-chemical processes complicating the direct application of the usual Chemical Engineering Plant Cost Index (CEPCI) approach for adjusting the costs to a new reference year). Tackling this is also the second cost scenario, which represents cost adjusted for the most costly technologies expected in the decade until 2030 reported in dedicated studies (see section S5 in the supplementary material) to show the expected development in the near-future (Table 3).

Table 3
Future cost scenario (2030) expected Capex reductions for the most costly technologies with respect to 2018 costs. The full set of costs with their reference can be found in sections S5 of the supplementary material.

Processes with adjusted costs	Capex reductions
Photovoltaics: north-south horizontal axis tracking	45%
Parabolic trough: north-south horizontal axis tracking	41%
Onshore wind turbine (3.0 MW)	19%
PEM water electrolyzer	67%
Direct air capture (DAC)	54%

Due to a relatively large computational resources needed, to solve the multi-objective optimization problem, no further uncertainty analysis with respect to the costs has been carried out at this point. The results of concrete process selection in the case studies should also be understood in this context as initial data points at an early stage of process development with realistic parameters gathered from other techno-economical studies, but which are still subject to uncertainty and would require further investigation into the identified designs to improve their conclusiveness on the path to technical realization.

In this context, one should also mention that the scaling of the investment costs (specific Capex) with production capacity of the processes is not considered as the focus was on including a large-enough time dimension to model the fluctuating nature of the renewable resource and storages. The effect of cost scaling, approximated with piece-wise linear functions, was investigated for model runs with lower number of typical days in a study presented in section S11 of the supplementary material, showing a large computational toll with only a small effect on the overall results.

2.6.2. Operation scenarios

It is uncertain if a large-scale industrial chemical production can be operated efficiently and safely with a constantly varying load copying the fluctuations of the renewable energy resources. Therefore, we vary the extent of operational flexibility of the methanol synthesis and purification processes. As one option we include an operation scenario where the minimum operational capacity ($minCAP$) of these processes cannot drop below 75% of the nominal capacity to model a conventional, stable operation of these processes. As a second option we include an operation scenario where the minimum operational capacity can drop to 0% to model a situation where these processes are allowed to flexibly adjust to the fluctuations fully. It is important to note that the used modeling approach cannot capture energy efficiency fluctuations for the overall methanol production within the operating window. Here, the necessary assumption of constant energetic efficiency across the operating window is supported by a dynamic modeling study showing a fluctuation of 1.7% between operation with hourly ramping rates at 100% and 50% of the installed capacity [81].

Comparison of the production costs of these two operation scenarios also highlights the overall incentive to operate these processes flexibly. On the other hand this also has an influence on the number of technologies being selected, since for the stable operation option a storage process needs to be installed to maintain the production capacity whereas flexible operation allows direct coupling to the fluctuations of the renewable energy sources and (at least for the one-hour time resolution considered in this study) exclude the installation of storage processes if not otherwise economically beneficial.

2.7. Model implementation and solution

The optimization problem has been implemented in GAMS (General Algebraic Modeling System). The most complex MILP optimization problem instances solved (using 10 typical days for standard designs) had on the order of 410 000 constraints, 170 000 continuous variables and 20 binary variables. The optimization problems were solved using the CPLEX solver utilizing the maximum number of threads (16) for parallel solution of the MILP problem, opportunistic search strategy, aggressive scaling strategy and probing, to name just a few of the solver settings (full settings can be found in the supplementary material of the GAMS model attached to this article). The logic for marking selected technologies using binary variables was implemented with indicator constraints of the CPLEX solver (which can be found within the full optimization problem in section S8 of the supplementary materials). Furthermore, extra binary variable constraints, determined based on process knowledge (e.g. knowing that at least one of the energy generation processes or at least one high-temperature heat source needs to be selected), were included to reduce the size of the MILP search tree and hence the computational time (section S8 of the supplementary material).

The model instances were solved on a computer cluster with computational nodes of 2x Intel Xeon Silver 4110 (Skylake) processors with 8 Cores per CPU and clock-rates of 2.1 GHz (3.0 GHz max). The model instances forming the individual Pareto fronts were solved in parallel on 10 of these nodes. Additionally, an initial guess solution (for the binary variable values) was input from model instances with lower number of typical days, which resulted in a significantly faster solution of the model instances with higher number of typical days. The computational times varied significantly based on the restrictions of the number of technologies being installed imposed through the ϵ-constraint method, with the most complex model instances taking more than 10 days to be solved.

3. Results and discussion

In this section the trends identified in the calculated Pareto fronts are reported first. Afterwards, the effects of standardization are described. The analysis of costs in the individual locations is carried out next, followed by the comparison of the results for different cost/operational scenarios, for which the cost increases due to standardization are calculated. Lastly, these cost increases are reflected on with the help of learning rates reported in literature for similar processes.

3.1. Pareto front trends

The Pareto fronts for the US case study are presented in Fig. 5 where the total annualized Capex for the designs in both of the considered locations are presented stacked on top of each other. The US case study with flexible operating scenario will be used to exemplify the general trends, which can be observed also in the Pareto fronts of the other scenarios (sections S9 and S10 of the supplementary materials). Generally, one can divide the Pareto fronts into 3 regions.

In the first region (from the most complex design with the maximum number of technologies until designs with 13 technologies being selected) the reduction of the number of technologies does not affect the combined production costs of methanol in the considered locations. Here one can identify the technologies, selected by the underlying optimization procedure, which contribute to the increased complexity of the design, but only add a negligible decrease to the production costs making them candidates to be removed from the design. These are not only technologies, which were selected with small installed capacities (Fig. 6) as a consequence of the applied linear optimization approach to the design problem, but also technologies selected in larger capacities (storage processes of TES at 714 °C, CO_2 and LOHC-NEC storage for H_2, heat pump to supply 65 °C heat), showing that significant parts of the design can be excluded with only a small increase in costs.

In the second region (from 13 until around 8 selected technologies) we start to see significant increases in production costs for each reduction of the numbers of technologies in the design. These represent the candidate designs, which should be considered in closer detail. Due to the inherent uncertainty of the cost parameters a final decision cannot be made based on the given parameters and rather the different candidates should be considered, even if their removal suggest a, now quantified, increase in the production costs relative to a more complex design. For the flexible operating scenario for example a design incorporating thermal solar energy generation (TS) a TES at 360 °C, with a heat engine utilizing the stored heat in periods of no renewable energy availability, is of interest (4.7% increase relative to the least costly/most complex design). However, an alternative design, which does not use parabolic troughs for thermal energy generation, but a system of TES at 714 °C, an electric boiler and a heat engine (operating between 400 and 145 °C) was calculated to be 6.8% more expensive. Such a cost difference may be offset by a more streamlined deployment of such a design and therefore should be among candidate designs for further investigation utilizing expert knowledge in the particular technologies. Nonetheless, if the cost-increases for the simpler designs start to become larger (e.g. >25%), the probability that the costs could be compensated by the simplification would be smaller.

The third region (below around 8 technologies being selected) represents designs, which are severely restricted in terms of the number of usable technologies where the costs rise sharply. In Fig. 5 the design using 7 technologies is restricted in such a way, that even wind turbines are not possible to be installed and therefore, the costs for the wind-dominant locations become extremely high as only PV panels are installed, resulting in a design, which is too simplified.

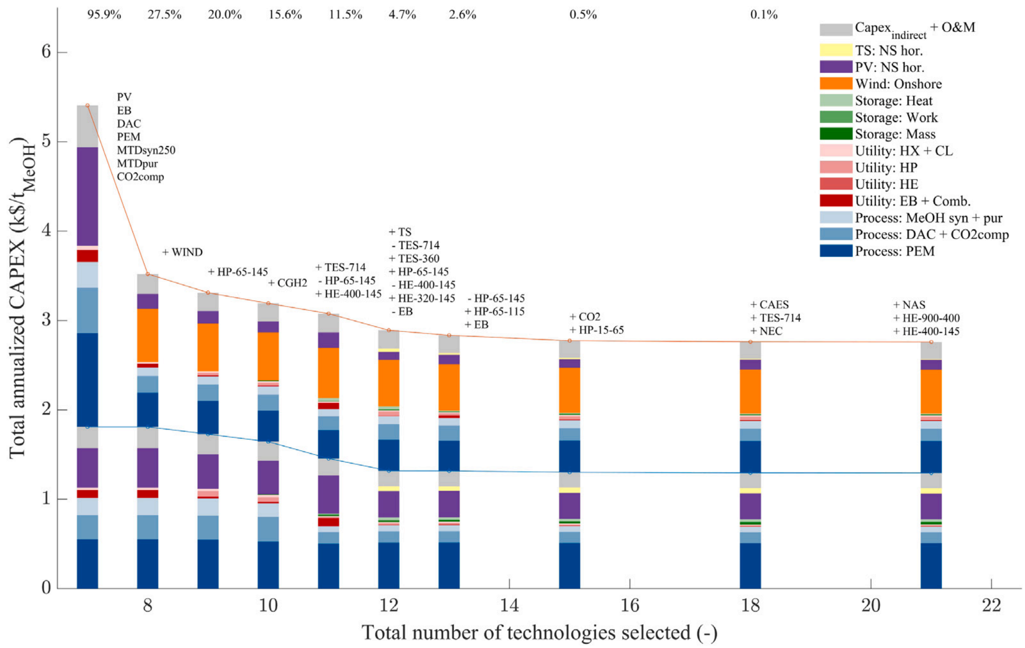
However, this is not only the case for such a unreasonable energy generation technology allocation, but the region starts sooner (<11 technologies) for the stable operation scenario (sections S9 and S10 of the supplementary materials). For stable operation the storage processes are essential to keep the methanol synthesis and purification processes running throughout the year as seen also on the larger contribution of storages to the total Capex in these designs.

On the other-hand for the flexible scenario, as the storage processes get excluded from the design we see increased installation capacities of the chemical processes (PEM, DAC, methanol synthesis and purification) as these begin to operate flexibly with reduced capacity factors (see Fig. 7) in order to reach the defined yearly methanol production capacity. Thus, the complexity is transferred from the complexity of design into the complexity of fluctuating operation implying a more elaborate control scheme. Additionally, one can see the usefulness of storage processes, not only to maintain a stable operating capacity defined by a technical limit of the chemical processes, but also to reduce the overall costs of production, a trend also observed in other studies for the Power-to-Methanol process [45,82].

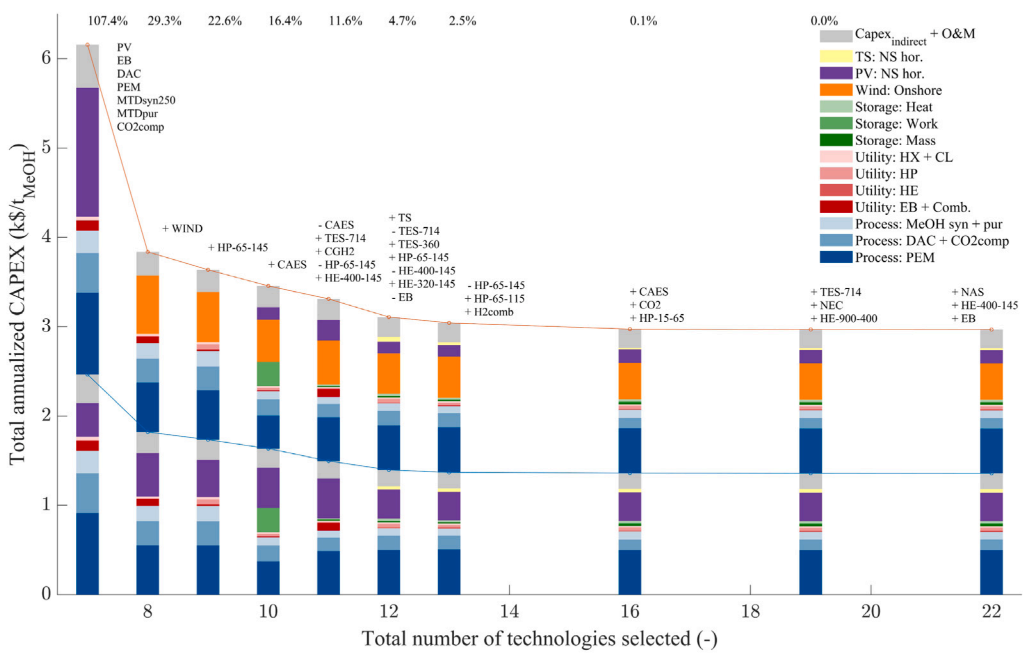
At this point one should also note one of the limitations of the proposed approach, where we limit ourselves to the number of different technologies installed as the proxy-measure for the complexity of the designs, which are determined by summing of the corresponding binary variables according to Eq. (12). Here it is implicitly assumed that each technology contributes the same level of complexity to the overall design. If more information is available, which would allow to evaluate the complexity contributions of the particular technologies relative to each other in detail (also considering different complexity measures on the level of the technology), one could incorporate this information into the proposed approach by assigning weighting factors to each technology (binary variable) considered. Nevertheless, using the exact approach presented in the case studies of this article together with the definition of a technology described in Section 2.1.2 should capture the binary nature of the benefits associated with reducing their total number described in Section 1.3.

3.2. Effects of standardization

Comparing the specific and standard designs, shows two important effects. The first one, as expected, the costs for the designs increases



(a) Specific design



(b) Standard design

Fig. 5. Pareto fronts for San Diego (bottom bars, blue line) - Kodiak (top bars, orange line) for flexible operating scenario and 2018 cost assumptions. Percentages at the top of the bar charts mark the delta of the total annualized Capex relative to the most complex design. The changes in terms of technologies being selected are marked above the bars going left to right (with + or − signs).

as standardization is imposed, due to the reduction of the degrees of freedom as the installed capacities of the major processing equipment are forced to be identical in both locations.

The second effect is that the standardization also influences the selection of technologies. One example of this is the design with 13 technologies (Fig. 6) where in the specific design the hydrogen combustion process (H2comb) is not selected, but in the standard design it is selected instead of the electric boiler (EB) for the production of high temperature utilities. This example shows only a relatively insignificant change to the overall design, as also shown by the fact, that the costs for hydrogen combustion or electric boiler processes only account for a small portion of the overall Capex (see Fig. 5) with the technologies serving only a supporting role in the design. A more pronounced influence of the standardization on process selection can be seen for the design with 10 technologies. Here the standard design is selected with compressed air energy storage for electricity (CAES) instead of compressed hydrogen storage (CGH2) in the specific designs (Fig. 6), resulting in a significant design change with larger cost contributions/roles of these technologies in the design.

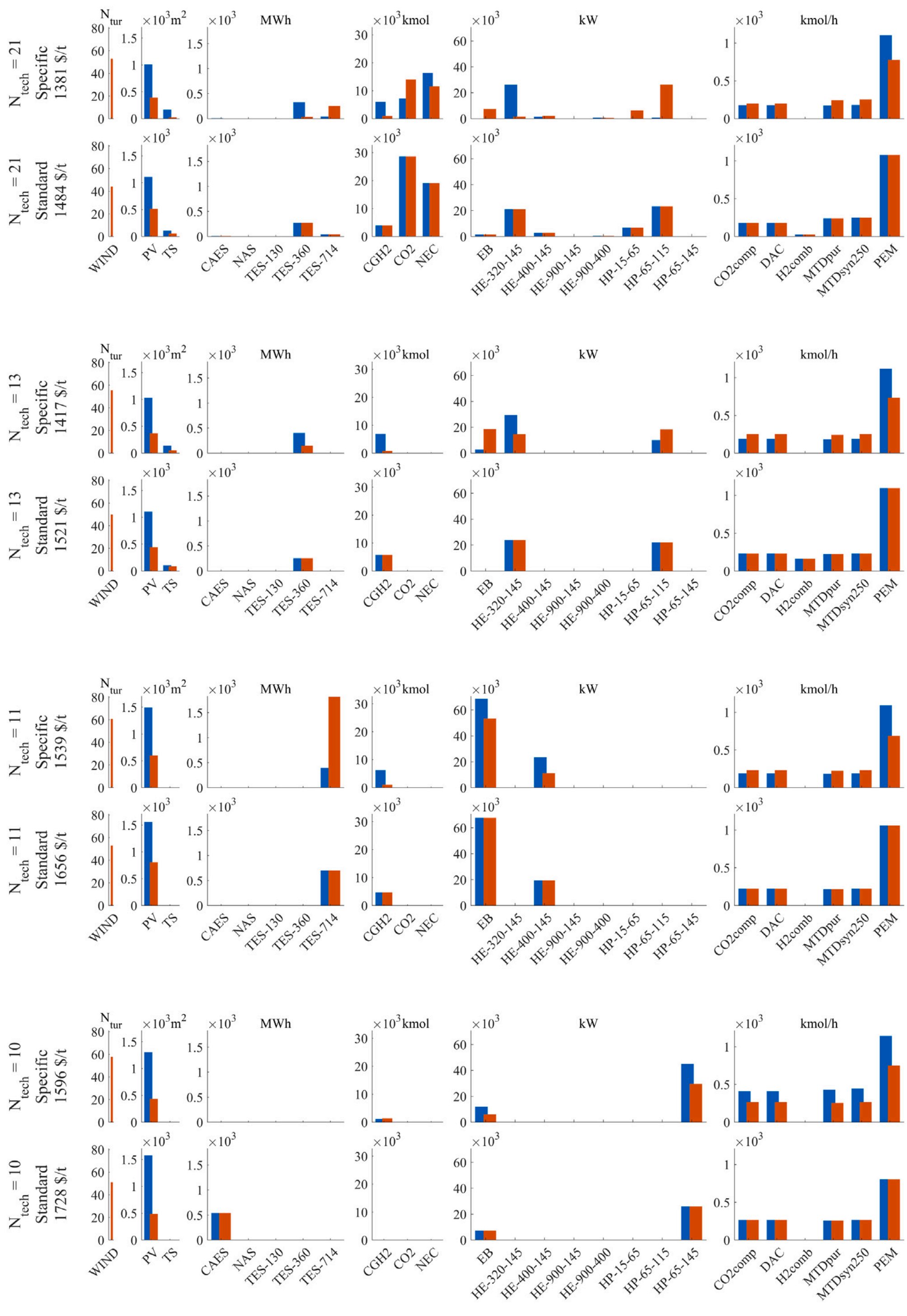


Fig. 6. Selected San Diego (blue) and Kodiak (red) designs with different levels of complexity and comparison of specific and standard designs for flexible operating scenario and 2018 cost assumptions with reported total annualized Capex per ton of methanol averaged across the two considered locations.

Nonetheless, the design with 13 technologies with hydrogen combustion in the standard design is an illustrative example for the need to consider the scheduling results when considering standardization across locations. Upon closer inspection of the average capacity factors of the hydrogen combustion process (Figs. 7 and 8), we see that the combustion process is not utilized at all in the San Diego location and is only forced to be installed by the standardization. Such useless installation of a technology should be prevented and can be identified by consulting the capacity factors and storage levels calculated from the scheduling results to see if the standardized processes serve a use in all of the locations.

However, the capacity factor and storage level figures (Figs. 7 and 8) show that this is an exception of a technology not being utilized at all (max. capacity factor equal to 0). Generally, even if standardization increased the installed capacities of a technology in one location significantly beyond the level identified in the specific design, the processes in the standard design reached their installed capacity during operation although some with a lower average capacity factors (with heat pump: 65–115 °C and heat engine: 320–145 °C being

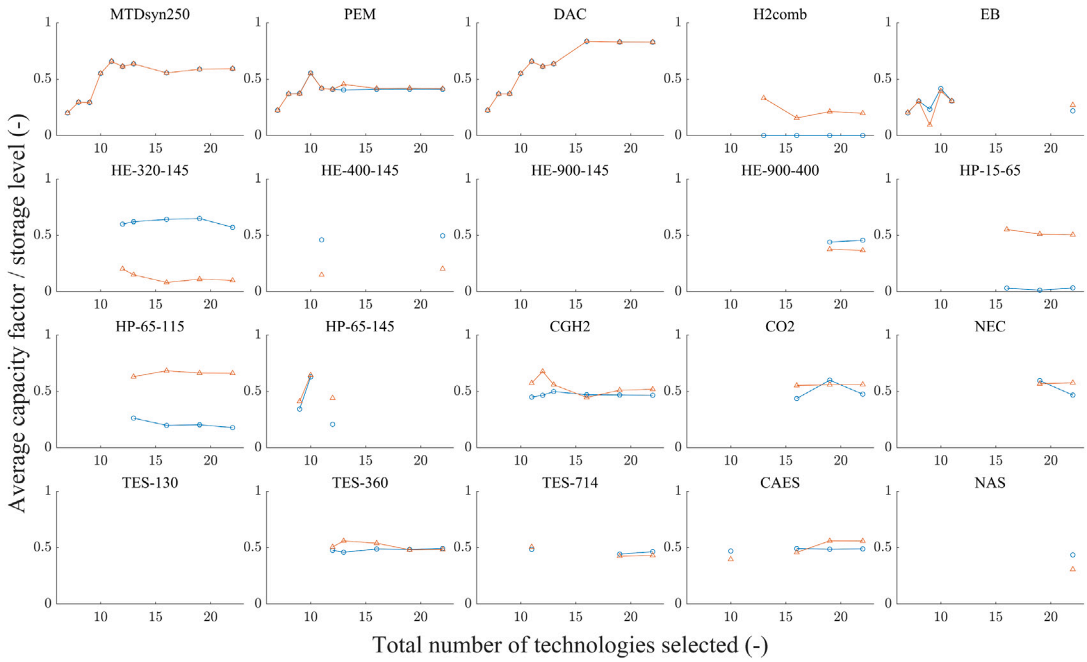


Fig. 7. Average capacity factors and storage levels for standard designs in San Diego (blue) and Kodiak (red) for flexible operation and 2018 cost scenario. Calculated as: average capacity factor (storage level) = average production capacity $\lambda_{(loc,p_{common},t_k,t_g)}$ (storage level $S_{(loc,c_{stor},t_i,t_{g+1})}$) in each hour throughout the year for each location divided by the maximum installed capacity $\lambda_{nom(loc,p_{common})}$ (storage capacity $S_{nom(loc,c_{stor})}$) across the locations.

the prime examples). This suggests that the extra installed capacities in the standard design versus the specific designs are still useful in both of the locations considered for standardization. Capitalizing on the lower average capacity factors in one of the locations for some of the technologies in the standard designs could be enabled by further research into finding complementary processes for co-production of other products together with methanol (sector-coupling), which would utilize these technologies when they are not required for producing methanol.

In Fig. 8 one can also see an interesting anomaly, which warrants explanation: the maximum capacity factor in both locations is lower than 1 for the methanol synthesis process with number of technologies below 10. This would suggest that the methanol synthesis process is unnecessarily over-sized in both of the locations, which should lead to sub-optimal solution. However, the reason for this is that the designs are so restricted in terms of the number of technologies, that these designs do not contain a storage process, which forces the methanol synthesis process to operate flexibly. Since the ramping limit (assumed as 30% per hour for the methanol synthesis process) is defined relative to the installed capacity (Eqs. (6) and (7)), the overall rate of ramping can be increased by increasing the installed capacity, showing the benefit of having higher (even than 30% per hour) ramping rates for designs without storage processes.

3.3. *Costs in the individual locations*

The trends of the Pareto fronts and the identified designs for the Chile case study (Fig. 9) are similar to the US case study, with the overall costs being lower, since the renewable energy conditions are better in Chile. However, comparing the costs in the individual locations (Table 4) sheds light on an important aspect of the considered standardization.

Firstly, the calculated costs are comparable with costs reported in previous studies of Power-to-Methanol systems [43,45] and still higher than the current market prices for the predominantly fossil-based methanol, even though that for the best location (Cabo Negro, Chile) and 2030 cost scenario the costs come within 11% of the price listed for the North American market (516 \$/t) [83].

Secondly, there is a strong asymmetric increase of production costs in the individual locations of the Chile case study when comparing the specific and standard designs. The costs in the wind-dominant location (Cabo Negro) are noticeably lower compared to the solar-dominant location (Mejillones). When the designs are standardized across these two locations, which do not have a comparable quality of renewable resources for methanol production (see the absolute value of the individual costs in specific design), the relative increase in costs due to standardization is high as the lower production costs achievable in an outstanding location are hindered by the worse location. We do not see such strongly asymmetric cost-increase differences in the US case study, where the locations are more comparable and where the solar-dominant location is the one, which can support the cheaper production of methanol.

This suggests that the selection of locations considered for standardization is important and opens the possibility for further research. In this respect the focus should lie on addressing the identification of representative locations (with associated renewable energy profiles) to base the standardization on. Here one should consider, if a location has common, wide-spread renewable resource conditions with a large market potential or a more rare outlier conditions, which can support only a small total production capacity. Such capacity limitation in these outstanding locations may arise also due to competition with other products requiring renewable resources as the industries will be shifting from fossil-based production.

3.4. *Comparing different scenarios*

Comparison of all the Pareto fronts for the different studied scenarios is presented in Fig. 10 showing the effect of methanol process flexibility and cost scenarios.

Immediately noticeable is the faster increase of costs with the reduction of the number of technologies in the stable operating scenario, as a consequence of the requirement for extra storage processes to keep processes operating stably. This also affects the relative cost difference between designs with different number of technologies installed operating either flexibly or stably (Table 5). For the most complex designs

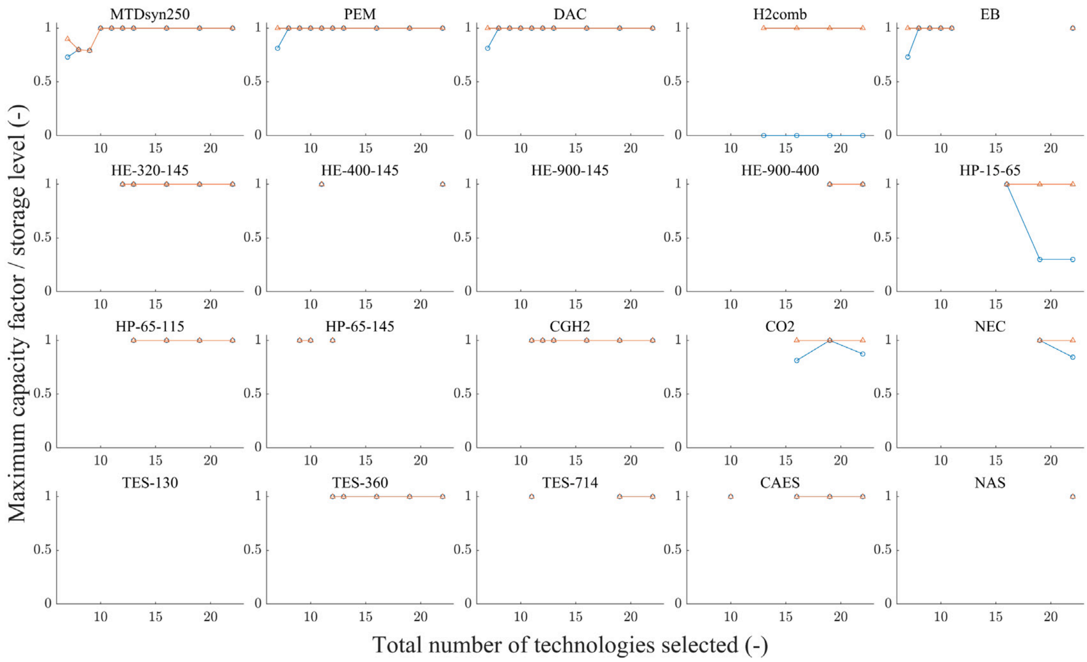


Fig. 8. Maximum capacity factors and storage levels for standard designs in San Diego (blue) and Kodiak (red) for flexible operation and 2018 cost scenario. Calculated as: maximum capacity factor (storage level) = maximum production capacity $\lambda_{(loc,p_{common},t_k,t_g)}$ (storage level $S_{(loc,c_{stor},t_i,t_{g+1})}$) in each hour throughout the year for each location divided by the maximum installed capacity $\lambda_{nom(loc,p_{common})}$ (storage capacity $S_{nom(loc,c_{stor})}$) across the locations.

Table 4
Total annualized Capex per ton of methanol produced in the individual locations for the most complex designs. The percentages mark the cost-increase due to standardization vs. specific designs.

Case	Costs	Operation	Design	Individual location TAC ($/t)	
				Solar dominant	Wind dominant
US	2018	Stable	Specific	1340	1556
US	2018	Stable	Standard	1410	1690
			Increase	*5.3%*	*8.7%*
US	2018	Flexible	Specific	1294	1467
US	2018	Flexible	Standard	1359	1609
				5.0%	*9.7%*
US	2030	Stable	Specific	709	945
US	2030	Stable	Standard	762	996
				7.4%	*5.3%*
US	2030	Flexible	Specific	661	870
US	2030	Flexible	Standard	714	926
				8.1%	6.5%
Chile	2018	Stable	Specific	1320	1020
Chile	2018	Stable	Standard	1357	1309
				2.8%	*28.3%*
Chile	2018	Flexible	Specific	1260	982
Chile	2018	Flexible	Standard	1308	1283
				3.8%	*30.5%*
Chile	2030	Stable	Specific	697	605
Chile	2030	Stable	Standard	724	740
				3.9%	*22.4%*
Chile	2030	Flexible	Specific	636	576
Chile	2030	Flexible	Standard	668	704
				5.1%	*22.3%*

Table 5
Comparison of costs changes for flexibility operation scenario (stable with respect to flexible scenario) for designs with different number of technologies (N_{tech}), case studies (US or Chile) and cost scenarios (2018 or 2030).

Design	N_{tech}	US 2018	Chile 2018	US 2030	Chile 2030
Specific	Most complex	5%	4%	8%	7%
	13	8%	9%	16%	16%
	10	29%	20%	35%	33%
Standard	Most complex	4%	3%	7%	7%
	13	8%	8%	16%	16%
	10	30%	19%	33%	30%

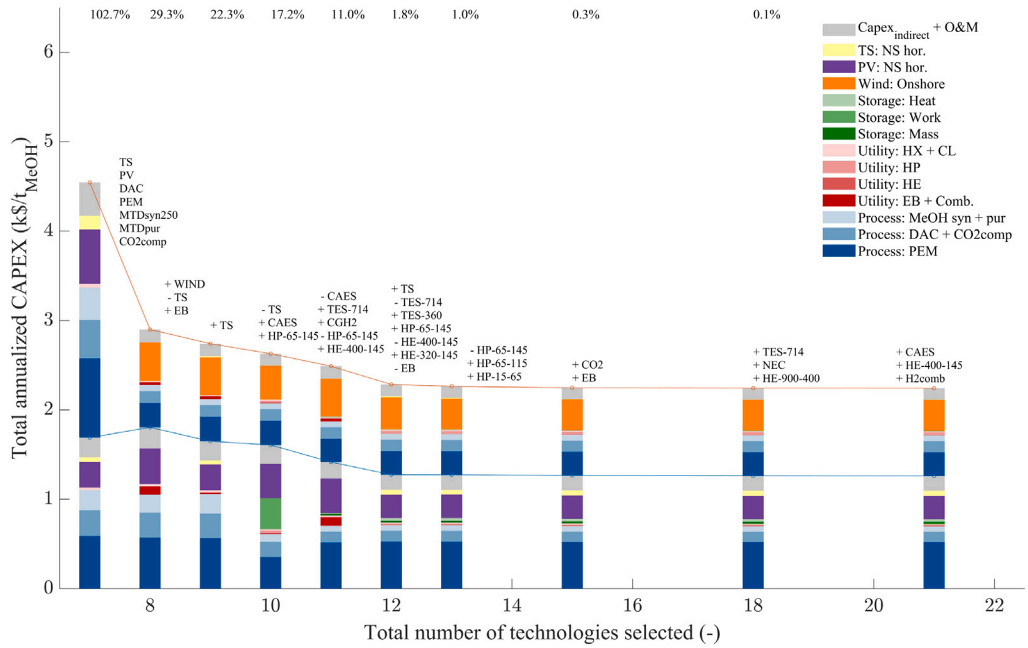
the cost-increases for stable operation amount to around 4% for both case studies with the 2018 cost scenario.

For the 2030 cost scenario, the difference between stable and flexible operation increases to roughly 7%, as the reduced costs of energy generation, the PEM electrolyzer and DAC represent a smaller part of the overall costs. This is also the case for designs with lower number of technologies, where we also observe the rising trend due to the reduced complexity, which predominantly affects designs with stable operation due to the requirement of storages to keep the processes running throughout the year making them more sensitive to complexity reduction.

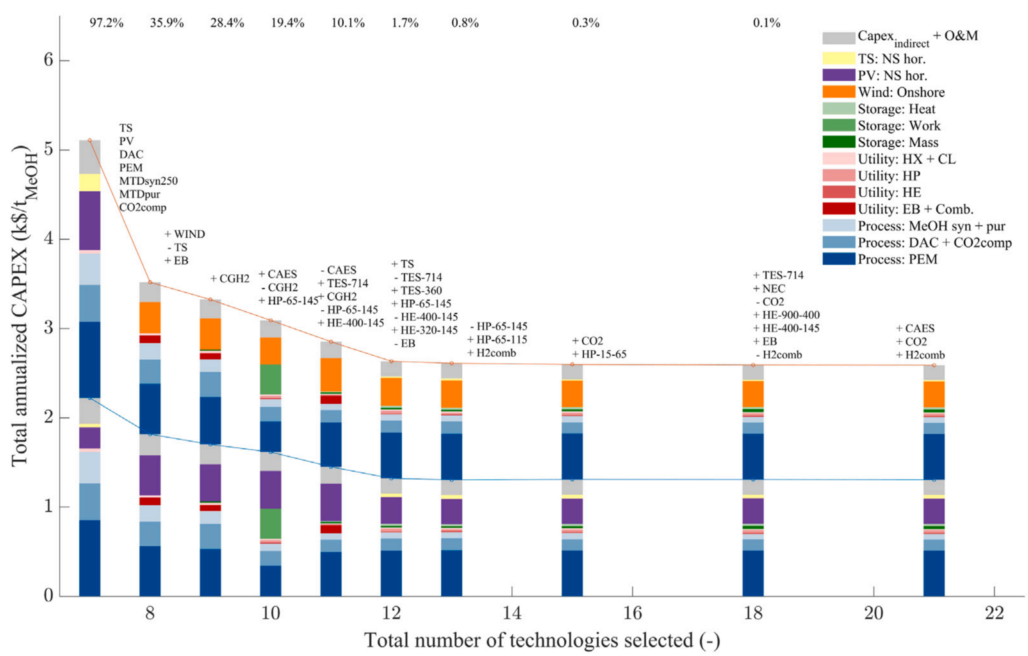
3.5. Costs of standardization

Fig. 10 shows the difference between the specific and standard designs, which is recalculated also into percentages of extra Capex due to standardization relative to the specific design to allow a better comparison. Here the costs are combined into an average Capex per ton of methanol produced as from the perspective of the engineering company offering such standardized plants, the Capex would be pooled together. These increases thus represent the extra costs due to standardization, which need to be compensated by the more efficient manufacturing/construction of the plants as a result of the economy of numbers.

In most of the scenarios a trend can be observed where for the designs with more than 10 technologies installed, there is a plateau of relatively constant Capex increases. These designs, weighted more towards lower production costs, would be prime candidates to be considered further. Hence the relatively constant cost-increases provide important information about the limits of cost reductions brought by standardization, which need to be reached in order to make it profitable. These can be used in a post-analysis considering the economy of numbers (Section 3.6).



(a) Specific design



(b) Standard design

Fig. 9. Pareto fronts for Mejillones (bottom bars, blue line) - Cabo Negro (top bars, orange line) percentages at the top of the bar charts mark the delta of the total annualized Capex relative to the most complex design. The changes in terms of technologies being selected are marked above the bars going left to right (with + or − signs).

To allow for a streamlined discussion of this post-analysis, and taking into account the underlying uncertainties, the values of these plateaus were taken as 7% for the US case study and as 15% for the Chile case study (marked in Fig. 11) with the slight variations between the individual designs of different scenarios ignored.

3.6. Learning rate analysis

The effects of the economy of numbers are often quantified by learning rate approaches [29,84–86]. To provide reference values to the broader literature on modular design and distributed production we estimate the required learning rates for the standard designs according to the one-factor approach described by the equations below [85]:

$$y = Ax^{-b} \tag{18}$$

where y is the cost of producing the xth unit, A the cost of the first unit, x the number of units or capacity, b the learning rate exponent, which is related to the learning rate R by:

$$R = 1 - 2^{-b} \tag{19}$$

However, one should account for the costs not only of the xth unit by itself when comparing alternative design concepts, but for the

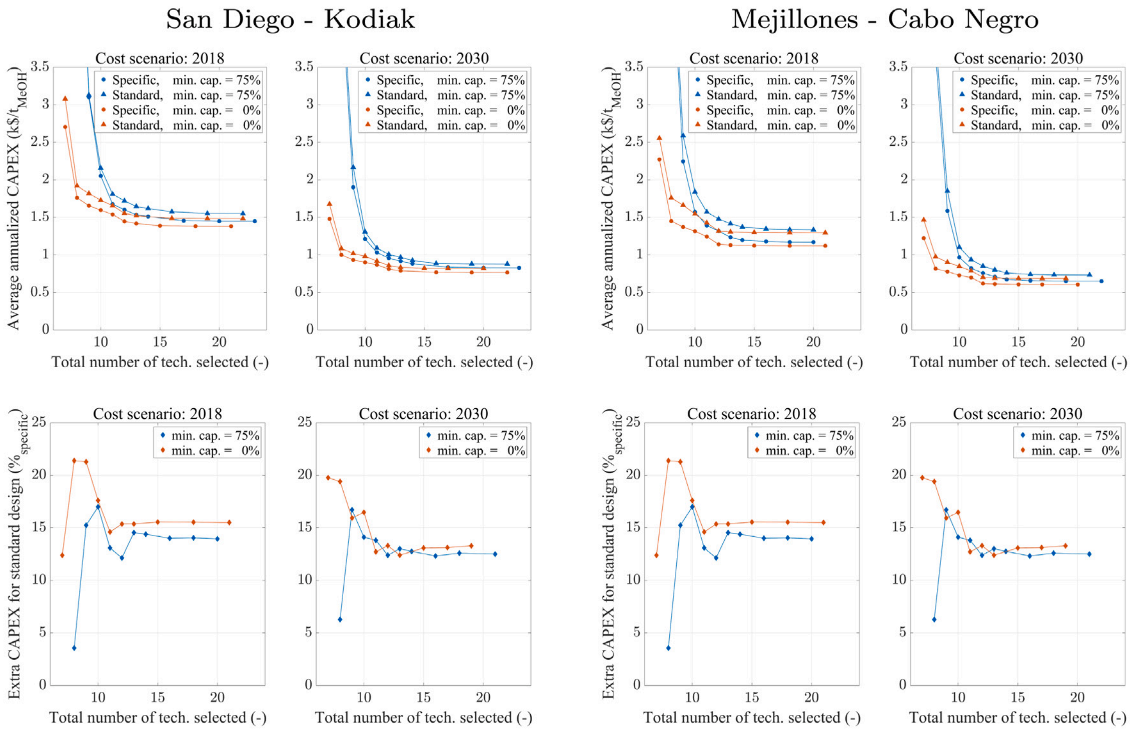


Fig. 10. Overview of Pareto fronts of all the scenarios (top row) and the calculated extra costs for standardization with respect to specific designs (bottom row).

cumulative cost reduction for the total number of units produced up until the xth (noted with N in the following equation). To also be able to compare the relative cost decreases, Eq. (18) was divided by the costs of the first unit A. As a result we get:

$$Y_{cumul,N} = \sum_{x=1}^{N} x^{-b}/N \tag{20}$$

where $Y_{cumul,N}$ is the learning effect multiplier relative to the costs of the initial unit, which accounts for the cumulative cost reduction up until N units are produced, with a given learning rate. Varying the total number of units produced N and the learning rate R results in the trends shown in Fig. 11.

To compensate the extra costs due to the loss of design flexibility as a consequence of standardization across the locations (7% for the US case study and 15% for the Chile case study) different learning rates (which would account for the reduction of costs to produce the plants and engineering) are required based on the number of plants produced (Fig. 11). As an example, a scenario where 20 plants of the proposed 40 000 t/y plants are produced (for reference this would represent 13.8% of the US and 0.8% of the world methanol market), an extra learning rate of 2.5% would be required to compensate for the extra standardization costs in the US case study with respect to an approach where all the plants are designed specifically for each location. For the Chile case study the learning rate would need to be 5.5%. These should be regarded as incremental changes to learning rates as a result of the standardization and not as absolute learning rates for specific technologies. Nevertheless, as a reference for the purposes of comparison we report these in the paragraph below.

Long-term learning rates for individual technologies can be found in literature [85] (e.g. mean values of 15% for gas turbines, 23% for solar PV, 11% for biomass power generation). Others report values of up to 10% for stick-built chemical plants considering just the construction learning and up to 20% when operational experiences are also included [87]. For modular plants, which are mass manufactured learning rates of up to 80% are even suggested [88] based on data from other manufacturing sectors [84]. Further learning rate estimates are based on the technology readiness level (TRL), which lead to learning rates of 10% for CO_2 capture and compression, 15% for CO_2 carbonation reactors or 5% for utilities in a CCU process [29]. Recommended learning rates are reported also by the National Renewable Energy Technology Laboratory of the U.S. department of energy for technologies similar to the ones found in the Power-to-Methanol process (3% for methanol and ethanol production, 5% for Fischer–Tropsch synthesis, 5% for hydrogen combustion turbines, 2% for H_2 production) [86].

Incremental increases to the learning rate as a result of a similar standardization as proposed in this work are however not reported, so it is not clear if the required learning rate increases can be achieved just as a result of deploying standard design across various locations with extremely different renewable resource conditions. Nonetheless, since the required learning rate increases are often lower than the absolute values reported for individual technologies, especially if fitting locations are paired together (US case study) or the market penetration would be high, it is possible that the overall process economics could be improved by the proposed standardization and warrants further investigation. This is also supported from another perspective considering modular plants, since Sievers et al. [89] report that engineering costs reduction due to standardization accounted for approximately 10% of the overall project costs reductions for a chlorine production plant project [90] and based on their own calculations confirm possible overall costs reductions to be between 6 and 11%.

In order to get better data regarding the possible cost reductions due to standardization, more intensive exchange with the industry is required with the aim to consult the internal experiences of EPC companies who have produced standardized plants to further elucidate the potential of such complexity reduction.

4. Conclusions and outlook

A method for the identification of simple and standard designs for the Power-to-Methanol process, which incorporates the fluctuations of the renewable energy resources with a large process network encompassing various waste-heat utilization pathways has been proposed. By application of the method a unique overview of alternative designs for the Power-to-Methanol process with different levels of complexity

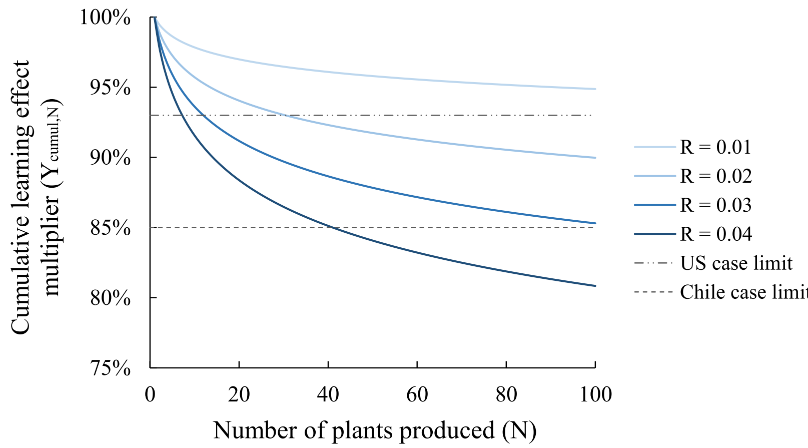


Fig. 11. Cumulative learning effect multiplier ($Y_{cumul,N}$) as a function of the total number of plants produced (N) and learning rate (R) with marked extra Capex limits needed to be reached to compensate the extra costs for standardization in the respective case studies.

is provided, allowing to make an informed selection into the most promising designs for further consideration.

By analyzing two different design pair case studies (one in the US and one in Chile) under different cost and operational flexibility scenarios, several important aspects regarding standardization and complexity reduction have been identified:

(1) The design complexity in terms of the number of different technologies can be reduced significantly compared to the most complex designs, initially identified by solving the underlying optimization problem not considering its complexity, with only negligible methanol production cost-increases, as shown by the Pareto fronts constructed in this study.

(2) For the most simple designs, the production costs can rise steeply as storage processes are excluded from the designs and the chemical and utility processes begin to operate flexibly with reduced capacity factors. This rise in costs is especially pronounced when the methanol synthesis and purification processes need to be operating stably throughout the year as in conventional chemical production of today. In other words, increasing the flexibility of these processes can result in production cost reductions (7% for the most complex designs in the 2030 cost scenario with an increasing trend as the number of technologies is restricted).

(3) Considering the identified designs: based on the considered cost scenarios, designs incorporating thermal energy storage, thermal solar energy generation, steam turbines and heat pumps utilizing waste-heat have featured in the Pareto-optimal designs, suggesting the importance of heat provision for the Power-to-Methanol process. Furthermore, standardization across different locations was shown to affect the selection of technologies compared to designs, which would be specifically designed for each location, showing the importance of including a broader process network in initial stages of process synthesis.

(4) The selection of locations with their specific renewable resource profiles to be considered for standardization is important. If two locations of different quality are paired together, the worse location can hinder achieving lower production costs in the better location and lead to strongly asymmetric production cost-increases in these locations, suggesting that these locations should not share a standard design.

(5) Standardization across wind and solar-dominant locations resulted in cost-increases due to the reduced design complexity of up to around 7% or 15% depending on the particular locations paired together for standardization. Especially, if fitting locations are paired together, the analysis of learning rates suggest that such cost-increases could be compensated for by the effects of the economies of numbers and reduction of engineering costs, making it of further interest for the scientific community and engineering companies focused on improving the deployment of Power-to-X processes.

However, more communication with industrial partners to get more specific data on achievable cost reductions through standardization and design simplification is needed. Crucially, the market demands need to be analyzed and stakeholders responsible for safety and environmental regulations in the deployment locations consulted, to see if the limited customization of the standardized designs could lead to a better competitiveness. Also the initial increase in design effort, already highlighted in this work by high computational resource requirement when solving the design problem for multiple locations at once, needs to be investigated further.

Additionally, of special interest for further research is finding methods, which can identify intermediate solutions for standardization while incorporating a higher number of different locations in parallel in the design problem. We have focused on identifying the worst-case scenario and important aspects related to standardization by pairing extreme locations (either solar- or wind-dominant) including a large process network. It is pertinent to ask, how would such a standardization perform for cases involving more than two representative design locations, which may incorporate locations with complementary solar and wind renewable resource conditions for example and how should the representative locations be selected? Would several standard designs emerge as the best solution, when a larger number of different locations is included, possibly considering also different demand profiles and interactions with other processes?

On the other hand, we have only applied the borderline design approaches in this exploratory study into standardization across locations (either fully specific designs for each location or a fully standardized design in both locations). Intermediate solutions, where only a subset of the processes in the process network would be standardized and other processes would be designed specifically for the particular locations, could offer Pareto optimal solutions in terms of standardization, especially if a higher number of representative locations are considered in parallel. Yet, to answer these research questions the modeling approach would need to be adjusted, and/or the process network simplified, as the computational resource requirement would be too large with the current approach considering a broad technological scope.

Such further research should be well supported by the results presented in this study highlighting the potential and pitfalls of complexity reduction, which suggest that even in the context of Power-to-Methanol process synthesis, everything should be made as simple as possible, but not simpler.

CRediT authorship contribution statement

Tibor Svitnič: Conceptualization, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft, Writing – review & editing. **Kai Sundmacher:** Funding acquisition, Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Simple PtM model (Original data) (Mendeley Data).

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the author(s) used GPT-3.5 from OpenAI in order to improve the quality of writing presented in this article in terms of grammatical correctness and stylistics. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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Appendix A. Supplementary data

The supplementary material includes an accompanying text to the main article as well as a folder containing the GAMS model file, together with the input data and results data presented in this article. Further data can be made available upon request.

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.enconman.2024.118325.

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