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IOP Conf. Series: Materials Science and Engineering **1301** (2024) 012132 doi:10.1088/1757-899X/1301/1/012132

Modelling and optimization of cryogenic mixed-refrigerant cycles for the cooling of superconducting power cables

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Abstract. For the green energy transition, the transport of large amounts of electrical energy is needed both in densely populated areas and over long distances. Superconducting power cables represent one possible solution, requiring energy-efficient liquid nitrogen re-cooling stations for an economical operation at cable lengths longer than about 1 km to 2 km.

In this contribution, a model for simulating cryogenic mixed-refrigerant cycles (CMRC) based on the Joule-Thomson effect and an associated optimization algorithm are presented. The distinctive feature of CMRC is the combination of good scalability of the cooling capacity, adaptability of the mixture to the specific application and an inexpensive process design. While the process is relatively simple, the identification of ideal operating conditions and mixture compositions requires complex modelling. In order to optimize these characteristics for CMRC processes, the Differential Evolution algorithm is adapted to a model built in Mathematica. Thermodynamic property data is calculated with the Peng-Robinson Equation of State as part of CoolProp, an open-source thermophysical property library. First simulation results are presented and further improvements are being discussed.

1. Introduction

To achieve the climate goals set by the Paris Agreement [1], whole sectors of the existing industry need to switch from fossil fuels to renewable energy. A much higher electrical energy demand is hence expected. Both the transmission performance needed and the age of current cables indicate the need for upgrading the existing power grid. Kottonau et al. [2] show the advantages of utilizing high temperature superconductor (HTS) cables in the power grid, yielding higher transmission performance with lower electric losses, no electromagnetic losses, no joule heating and a lower space demand. Especially the latter makes HTS cables an interesting candidate for updating the power grid in densely populated areas such as urban centers. This is the goal of the SuperLink project, to prove the feasibility of introducing a 110 kV, 500 MVA connection in the city of Munich, Germany [3]. The SuperLink cable will be 12 to 15 km long, making it the longest HTS cable within a power grid.

To enable operation of this technology within the energy sector, HTS cables need to be cooled permanently. As in most HTS applications, the SuperLink cable uses liquid nitrogen (LN_2) as coolant. Due to pressure losses and heat inleak, multiple cooling stations along the length of the

cable are needed, where the pressure drop is compensated by pumping and the LN_2 is sub-cooled again to the entry temperature.

Different technologies are available to provide the cooling power. The concept applied in the AmpaCity project [4] uses vacuum pumps to sub-cool the LN_2 in an open circuit, requiring a steady LN_2 supply. In the considerably longer SuperLink cable, however, an open process is not foreseen by the grid operator. A theoretical alternative is the use of regenerative cooling processes, such as Stirling coolers, but their cooling power limitation does not fit well to the required 30 kW at 70 K. Technically and economically interesting alternatives are found in the group of recuperative cooling cycles. One option is the (reverse) Brayton cycle, which is highly efficient due to the use of cold turbo-expanders. Another option is the cryogenic mixed-refrigerant cycle (CMRC) based on the Linde-Hampson (LH) process, using wide-boiling fluid mixtures with compositions adapted to the application. In comparison to the Brayton cycle, CMRCs bear the potential of being less expensive (no cold turbo-machinery) and more compact (higher power density due to the phase change of higher boiling components). A competitive efficiency, however, needs to be demonstrated in view of energy consumption and operating cost.

To reach the needed temperature level of around 70 K for cooling HTS power cables, it is advisable to use a multi-stage process in form of a CMRC cascade. Single-stage processes become inefficient at such low temperatures, since the percentage of high-boiling mixture components needs to be reduced to prevent freeze-out [5]. In this contribution, we focus on the development of a simulation model of the CMRC and an algorithm to optimize the refrigerant mixture for a specific use case. The aim is to build a model for a CMRC cascade, but as a first step, a single-stage simulation and optimization is presented.

2. Process modeling

Figure 1 shows a single-stage CMRC, signifying the simplest possible process design to reach low temperatures. The performance is predominantly defined by the properties of the working fluid. Compared to pure refrigerants such as nitrogen, neon or helium, the use of wide-boiling mixtures considerably widens the parameter space for optimization (number and kind of components, concentrations), beyond the operating temperatures, pressures, flow rates and capacities. Therefore, a model is being developed that can be executed on a high-performance computing (HPC) cluster using Mathematica [6], to find the theoretically ideal mixture for an application. As the modeling of mixture properties implies large uncertainties, the pre-selection must be validated experimentally at a later stage. As equation of state (EoS), the Peng-Robinson EoS is chosen, representing mixture behavior better than other EoSs [7]. The Twu α function [8] is used with values from Bell, Satyro and Lemmon [9]. Binary interaction parameters are taken from Aspen Plus [10]. For thermodynamic property calculations, the open-source library CoolProp [11] is used[1].

2.1. Assumptions and boundary conditions

The model presented in this work is designed as a framework for mixture optimization, using several simplifications. This includes a constant compressor efficiency, the pre-definition of minimum temperature differences and pressure losses, and the ideal thermal insulation of components. The goal of the cycle calculation is to find the energy demand of a given process, requiring the thermodynamic state before and after each component. Known or given temperatures are defined at the outlet of the ambient aftercooler (AC) $T_{\mathrm{AC,out}}$, and at the inlet and the outlet of the cooler ($T_{\mathrm{cooler,in}}$, $T_{\mathrm{cooler,out}}$).

[1] To facilitate the use of CoolProp, several contributions were made to the open-source project `https://github.com/CoolProp/CoolProp`, and the Mathematica wrapper was expanded to include more functionality.

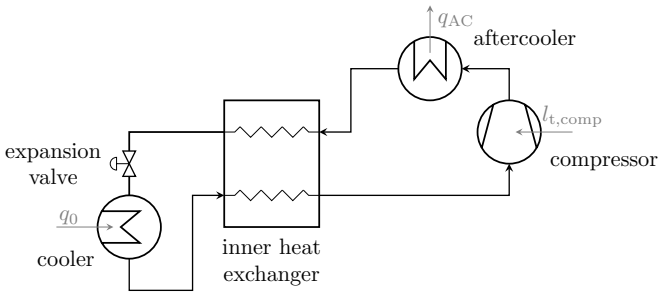

Figure 1. Single-stage cryogenic mixed-refrigerant cycle.

2.2. Process parameter calculation

In a simulation, all pressure values are set first, defining high and low pressure levels (p_{HP}, p_{LP}) and the pressure drops Δp_i in the components. Next, the temperatures are defined for the AC outlet, the cooler inlet and outlet, and the corresponding porperty calculations are performed. With the AC outlet enthalpy, the entry state of the HP passage of the inner heat exchanger is calculated. The expansion inlet and the HP outlet of the inner heat exchanger are derived from the cooler inlet enthalpy, assuming isenthalpic expansion. The LP inlet enthalpy to the inner heat exchanger corresponds to the cooler outlet enthalpy. With an energy balance around the inner heat exchanger, the outlet of the LP passage and the remaining states (compressor inlet and outlet as well as the AC inlet) are calculated.

To ensure the refrigerant flow not entering the compressor in a two-phase state, the entry is checked to be at least $\Delta T_{superheat}$ above the dew temperature of the refrigerant mixture. If this is not the case, heat is added with a heater, whose energy demand is added to the energy demand of the process.

Further, it is possible to enable the lowering of $T_{cooler,out}$ to include mixtures that would have a pinch point at either end of the inner heat exchanger with the original values. The lowest $T_{cooler,out}$ can be set is $T_{cooler,in}$, which would result in $h_{cooler,out} = h_{cooler,in}$ and thus no transferred heat. Due to the refrigerant being a mixture, it is highly unlikely there would be a constant temperature phase change. If the lowest $T_{cooler,out}$ still results in a pinch point, the original value is reinstated and a penalty is calculated as explained below.

2.3. Heat exchanger modeling and pinch point detection

One objective of CMRC optimization is the matching of heat capacity flow rates within the hot and cold passage of the inner heat exchanger, yielding smaller temperature differences and lowering the energy demand of the overall system. At the same time, this also poses the threat of pinch points inside the heat exchanger, which can lead to temperature profiles intersecting each other in the simulation. To prevent this unphysical behavior from producing wrong results, pinch points and temperature intersections are recognized and quantified. For this purpose, the temperature profiles are calculated at discrete points along the heat exchanger. For each passage, the transferred heat is calculated when reaching a certain temperature, which is increased by a given step size. If a step were to overstep a phase transition, the step is shortened to include the bubble/dew point. Since this model does not include dimensioning of heat exchangers, the pressure drop is assumed with a simple estimate, which could be subject to change in future versions. For single-phase flow, the pressure drop is evenly spread over the temperature change. Within the two-phase region, the pressure drop is evenly spread over the vapor quality change.

Kochenburger [7] developed an algorithm for the successive elimination of temperature intersections, which includes a quantification of the unphysical behavior according to eq. 1. It calculates the surface area A between the temperature profiles in the region, where the

temperature difference is negative or lower than a given $\Delta T_{\mathrm{min,HX}}$

$$A = \int_0^{|\dot{Q}_{\mathrm{total,HP}}|} \max\left\{0, \Delta T_{\mathrm{min,HX}} - (T_{\mathrm{HP}} - T_{\mathrm{LP}})\right\} \mathrm{d}|\dot{Q}_{\mathrm{HP}}| \tag{1}$$

with HP and LP representing the high- and low-pressure stream, respectively. The calculated value is used in the optimization as parameter for a penalty function (cf. section 3.2, eq. 3) to punish unphysical results.

3. Mixture optimization

As the thermodynamic property data calculated in the process simulation is imported from an external library and the relations within the system cannot be represented by a set of equations, it is not possible to calculate gradients with the model. Thus, when selecting an optimization algorithm, one must ensure that derivatives are not needed. Furthermore, the algorithm should find a global optimum independently of initial values. These features are provided by the "Differential Evolution" (DE) algorithm from the group of genetic algorithms, which was first proposed by Storn and Price [12].

3.1. Differential Evolution algorithm

Instead of a single starting value, DE has a fixed-size population of *Np* candidates, which are mutated and combined in individual generations to form new candidates that are compared with the previous ones. The population remains the same size during the whole algorithm, initially exploring the parameter space through a broad distribution of initial values and later converging closer and closer towards the optimum.

Initialization The candidates for the initial population are either randomly generated or created using a grid pattern for all input parameters, and the target value is calculated for the whole population. A big population with a broad distribution over the parameter space should prevent the algorithm from converging on a local optimum.

Generation The initialization is followed by the optimization, which is performed in the form of generations. For each candidate of the current population, all the subsequent steps of mutation, recombination and selection are carried out, before the next generation starts, enabling parallel computation. In the following, a generation for a single candidate x_i from the population $\{x_1, x_2, ..., x_{Np}\}$ is described. All candidates x are to be understood as vectors, whose individual elements determine the parameters of the respective calculation.

- *Mutation* First, three candidates different from x_i (x_{r0}, x_{r1} and x_{r2}, $r0 \neq r1 \neq r2$) are selected and combined by eq. 2 to form mutant v_i

$$v_i = x_{r0} + F \cdot (x_{r1} - x_{r2}) \tag{2}$$

  where F is the scale factor that determines how far v_i deviates from x_{r0}.
- *Recombination* Next, the mutant v_i is recombined with the current candidate x_i to form u_i, individual parameters of the respective vectors are randomly selected as illustrated in figure 2. The crossover probability *cr* controls how likely a parameter is taken from either v_i or x_i. By randomly selecting one of the parameters beforehand, for which the mutant value must be taken, it is guaranteed that u_i will be different from x_i.

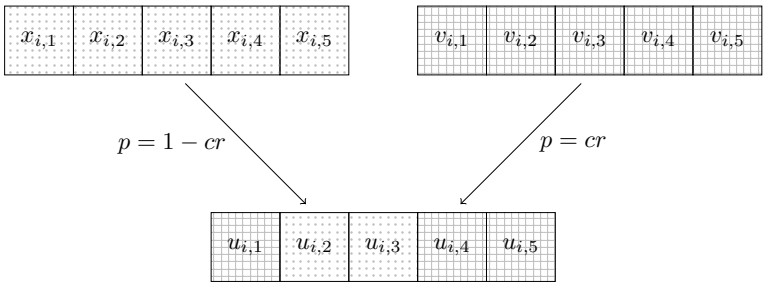

Figure 2. Schematic depiction of recombination step.

- *Selection* Before the target value is calculated, it must first be verified that u_i satisfies given boundary conditions. If this is not the case, the candidate is adjusted accordingly. Subsequently, the calculation is performed and possible penalty functions are applied. After comparing the results of the new and the old candidate, the better candidate remains in the population.

Abort criteria When all candidates have either remained in the population or have been replaced by new ones, termination criteria are checked at the end of a generation. If one of these criteria is fulfilled, the algorithm ends and – in case of convergence – the optimum is found.

3.2. Application of DE on CMRC simulation

For now, the goal of the optimization is to find the optimum mixture composition in combination with the pressures (p_{HP}, p_{LP}); all other operating parameters could also be subject to optimization. To apply the DE algorithm on the CMRC model in section 2, the algorithm is adapted as follows:

Initialization For the initial population, *Np* composition and pressure vectors are created. The pressures are random values in between given pressure boundaries for each p_{HP} and p_{LP}.

The molar composition can be created by generating m random numbers between 0 and 1, m being the number of components in the mixture. As the total of this composition is most likely not equal to 1, the composition is normalized. This, however, is prone to producing few candidates with extreme compositions like 0.1 of one component, 0.9 of another component and (almost) nothing of the remaining components. This can be mitigated by generating the population on a grid, where all candidates are binary mixtures of all possible combinations, ranging from one extreme (0:1) to another (1:0). The step width depends on the number of candidates *Np* needed. After generating the initial candidates, boundary checks are performed for the candidates single component compositions. If one or more components of a candidate are out of bounds, the components' fraction is set to the violated boundary and the remaining fractions are normalized to reach a total of 1.

Next, all candidates are passed in parallel computation to the simulation, where the power input (compressor and heater) is calculated for all candidates. For each candidate x_i the temperature profiles are generated and the inner heat exchanger is checked for pinch points (see eq. 1). If the calculated area A is larger than 0, the following penalty function is applied to the calculated power input l_{t}

$$\tilde{l}_{\mathrm{t}} = l_{\mathrm{t}} \cdot e^{\psi \cdot A} \tag{3}$$

where ψ is the penalty value. If a candidate's simulation did not terminate without error, this candidate $x_{i,\mathrm{failed}}$ needs to be replaced by a new one. A new random candidate $x_{i,\mathrm{random}}$ is

generated and eq. 4 is used to create the new candidate $x_{i,\text{new}}$

$$x_{i,\text{new}} = 0.8 \cdot x_{i,\text{failed}} + 0.2 \cdot x_{i,\text{random}}. \tag{4}$$

This ensures the new candidate is related to the original failed candidate, which keeps a broad initial distribution.

The calculation, penalization and regeneration of initial candidates is repeated until either the needed number *Np* of candidates was successfully initialized, or a maximum number of repetitions was performed. In the latter case, the algorithm will abort and no optimization is run.

Mutation and recombination The mutation and recombination steps are performed as described in subsection 3.1.

Selection Before simulating the new candidate v_i, it must be checked whether it is within the boundaries given to the algorithm, and whether the component concentrations sum up to 1.

- To abide to the given boundaries, but prevent the algorithm from driving the optimization towards these boundaries, Price, Storn and Lampinen [13] recommend setting the violating entries to the midpoint between the *base* candidate (x_{r0} during mutation, see eq. 2) and the boundary.
- After "fixing" the entries with violations, the remaining component concentrations are normalized to a total of 1.
- If no boundaries are violated in the first place, the composition is normalized.
- Should, in either case, normalization violate the boundaries for another component, the algorithm is run (again).

Next, the simulation is run, the power input (compressor and heater) is calculated for v_i and temperature profiles are generated. In case of pinch points, the penalty function (cf. eq. 3) is applied. The (penalized) power value $\tilde{l}_\text{t}$ for u_i is compared to the value for x_i and the better candidate remains in the population. Should an error occur during any of the calculation steps (numerical error in Mathematica or an error from CoolProp) x_i automatically remains in the population.

Abort criteria After each generation the following abort criteria are checked:

- convergence (difference between all candidates and best candidate smaller than ε)
- maximum number of generations
- abort time (for optimizations run on HPC hardware)

If a criterion is met, the initialization values, the current values and all generations in between are saved for analysis. The model also saves these values in case of a user-triggered abort. If no abort criterion is met, the next generation is run.

4. Results and discussion

In order to demonstrate the capabilities of the current model, an optimization with a small parameter set is carried out on bwUniCluster 2.0 [14] for a single-stage CMRC. To see the difference in optimum composition for different cooling temperatures, $T_{\text{cooler,in}}$ is varied between 90 to 150 K in increments of 1 K. Component concentrations of propane, ethane, methane and nitrogen are subject to the optimization algorithm, while pressures and other operating conditions are held constant. The process simulation parameters are listed in table 1, and the

Table 1. Boundary conditions and assumptions for single-stage CMRC optimization.

Boundary condition	Symbol	Range/Value
high pressure (HP)	p_{HP}	16 bar
low pressure (LP)	p_{LP}	4 bar
ambient temperature	T_{ambient}	293.15 K
minimum temperature approach in aftercooler (AC)	$\Delta T_{\mathrm{min,AC}}$	5 K
cooler inlet temperature	$T_{\mathrm{cooler,in}}$	90–150 K
cooler outlet temperature	$T_{\mathrm{cooler,out}}$	$T_{\mathrm{cooler,in}} + 5$ K
minimum temperature approach in inner heat exchanger	$\Delta T_{\mathrm{min,HX}}$	2 K
minimum super heated temperature at compressor inlet	$\Delta T_{\mathrm{superheat}}$	2 K
isentropic compressor efficiency	η_{is}	0.7
pressure drop for component/pipe i	Δp_i	1000 Pa
molar composition of refrigerant mixture	x_i	0–1

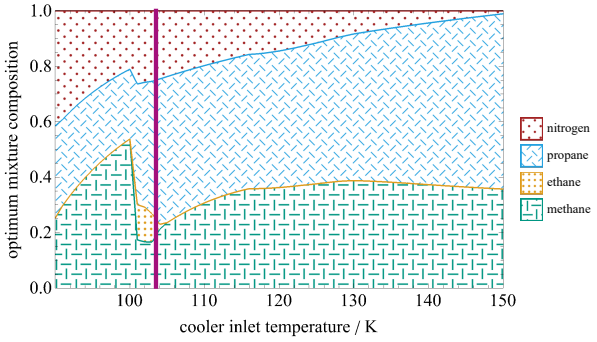

Figure 3. Change in optimum composition over different $T_{\mathrm{cooler,in}}$.

Table 2. Optimization parameters.

Optimization parameter	Symbol	Value
number of candidates	Np	70
convergence criterion	ε	0.00001
scale factor	F	0.5
crossover probability	cr	0.5
penalty factor	ψ	100

optimization parameters in table 2. The initialization is run with the population on a grid for all possible binary combinations. The cooler outlet temperature $T_{\mathrm{cooler,out}}$ is not varied to mitigate pinch points; it is kept at $T_{\mathrm{cooler,in}} + 5$ K.

Figure 3 shows the change in the optimum composition for different $T_{\mathrm{cooler,in}}$. Below 104 K left to the vertical line in Fig. 3, the algorithm does not find compositions without intersection of the temperature profiles in the inner heat exchanger. This is caused by the relatively low pressure ratio, leading to a lack of cooling power provided by the Joule-Thomson effect. The existence of temperature intersections and pinch points explains the very different compositions for the cooler inlet temperature range of 90 to 103 K.

For the physically possible optima right to the vertical line in Fig. 3, the amount of methane reaches a maximum at $T_{\mathrm{cooler,in}} \approx 130$ K . Ethane is forced out of all optima, except for $T_{\mathrm{cooler,in}} = 104$ K, while propane is the main component in all optimum mixtures. The nitrogen concentration is about 25 % at the lowest possible temperature, being steadily replaced by propane at higher temperatures.

5. Conclusions and outlook

A tool for the mixture optimization in cryogenic mixed-refrigerant cycles (CMRCs) is presented. The principle of the applied Differential Evolution (DE) optimizer is explained and the results of example calculations are shown for a single-stage CMRC process. The simulation model and

the optimization algorithm are implemented in Mathematica, and thermodynamic property data are calculated with the Peng-Robinson EoS available in CoolProp. The example optimizations illustrate the functionality of the developed algorithm for a reduced parameter set.

The optimization parameters need further investigations to make the calculations more efficient. Besides the number of candidates, convergence criteria, scale factor and the crossover probability, especially the penalty function needs a closer inspection. Another aspect that will be investigated is the selection step. While here the candidate u_i is directly compared with the old candidate x_i (One-to-One Survivor Selection), other selection schemes are available, where e.g. the worse candidate can remain in the population with a certain probability (to escape local optima), or all candidates, old and new, are ranked together and only the Np best remain in the population [13].

Beyond the single-stage Linde-Hampson (LH) process presented in this paper, the model is being further developed for CMRCs with phase separators (auto-cascades) and for CMRC cascades. A more advanced single- and multi-stage compressor model will also be implemented. The tool will then be applied to identify an optimum CMRC design for the cooling stations in the SuperLink project. Following a detailed component design for the optimized process parameters, the potential of the CMRC technology will be assessed in comparison to reverse Brayton coolers.

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Acknowledgments

The authors would like to acknowledge the support by the state of Baden-Württemberg through bwHPC and from the Karlsruhe School of Elementary Particle and Astroparticle Physics: Science and Technology (KSETA).