CHEMICAL ENGINEERING TRANSACTIONS

VOL. 39, 2014

A publication of AIDIC
The Italian Association of Chemical Engineering
www.aidic.it/cet

Guest Editors: Petar Sabev Varbanov, Jiří Jaromír Klemeš, Peng Yen Liew, Jun Yow Yong

ISBN 978-88-95608-30-3; **ISSN** 2283-9216

DOI: 10.3303/CET1439191

Methodology for Identification of Suitable ORC-Cycle and Working-Fluid using Integration with Multiple Objectives

Matthias Bendig*[a], Daniel Favrat[b], Francois Marechal[a]

[a]Ecole Polytechnique Federal de Lausanne, STI IGM, Industrial Process and Energy Systems Engineering (IPESE) / Industrial Energy Systems Laboratory (LENI), Station 9, 1015 Lausanne, Switzerland
[b]Ecole Polytechnique Federal de Lausanne, Energy Center, EPFL IV CEIF CEN, BAC 104 (Château En Bassenges), Station 5, 1015 Lausanne, Switzerland
matthias.bendig@epfl.ch

In recent times the interest in electricity production with Organic Rankine Cycles (ORC) has increased. A look into recent publications shows that the identification of suitable working fluids is in general done by a look at a more or less small number of fluids and a predefined type of cycle (single-stage, two stage, trans-critical etc.).
In this publication we describe a methodology that is capable of choosing the design-point, a suitable working fluid and a type of cycle. This is done while in parallel integrating the cycle with any process, using composite curves and pinch analysis.
The methodology proposes a multitude of decision criteria for the optimal cycle which are either thermodynamic criteria like exergy efficiency, energy efficiency, maximum or minimum pressures and temperatures, or economic criteria. Additionally it is possible to include qualitative and quantitative criteria to make a pre-selection e.g. Toxicity, Global Warming Potential (GWP) and Ozone Depletion Potential (ODP).
We propose a new methodology, as shown in Figure 1, using a genetic algorithm for the multi objective optimisation (Master-Problem) of suitable ORCs with available heat sources and MILP (Slave-Problem) for fitting of the cycles. The crucial point of this methodology is the choice of the cycle within the MILP-Slave Problem. This means that all possible fluids are tested for a set of thermodynamic parameters and the best one regarding the chosen selection objective is send back to the Master-Problem for evaluation. This has the advantage of testing all fluids within a limited time frame.

1. Introduction

The use of low temperature (waste) heat for electricity production is limited on one side by the low exergetic potential (Borel and Favrat, 2010) of the heat sources and by the difficult economic environment on the other side. High investment cost (Lazzaretto et al., 2011) in suitable technologies and low electricity prices for industry in many parts of Europe and the world, accentuate this. This makes careful studying of all options necessary, including proper integration with the process. Identifying the right cycle to integrate with an industrial process depends firstly on the real waste heat potential found in the process, identified with the methods described in (Bendig, 2012) and in more detail in (Bendig, 2013). Once the potential has been quantified and qualified, a methodology can be applied to systematically identify adapted cycles for electricity production.
The identification is difficult for numerous reasons, there is a large number of possible working fluids, the design of the cycle itself can have different forms (stages, extraction etc.) pressure and temperature levels for a given fluid and cycle can be varied largely additionally the equipment to use can have different forms and materials. In recent papers similar analysis have been done by choosing a more (Maraver et al., 2012) or less (Heberle et al., 2012) large number of fluids and testing them with different parameters (Schuster et al., 2009). With the methodology proposed in this paper, we want to address some of these difficulties,

Please cite this article as: Bendig M., Favrat D., Marechal F., 2014, Methodology for identification of suitable ORC-cycle and working-fluid using integration with multiple objectives, Chemical Engineering Transactions, 39, 1141-1146 DOI:10.3303/CET1439191

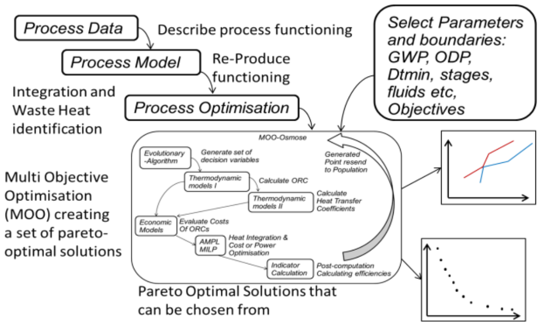

Figure 1: Cycle identification embedded in Integration

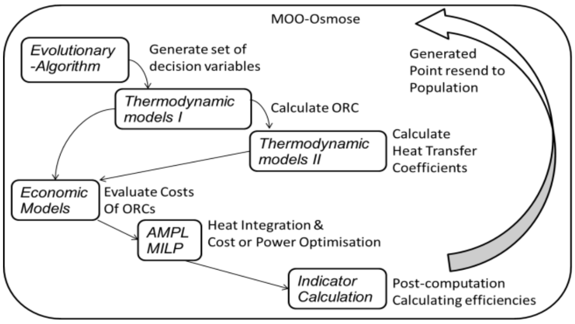

Figure 2: Multi-Objective-Optimisation Algorithm

analysing at the same time economic factors and thermodynamic factors with a methodology that allows for multiple fluids. In the following we will describe the main steps which are involved.

2. Method description – Multi-Objective-Optimisation

The methodology is based on a prior identification of the real waste heat potential (Bendig, 2013) of an industrial process. The resulting composite curves will be used for the integration of the low temperature electricity production cycle (LTHC) (Figure 1). The identification of suitable cycles is done with a Multi-Objective-Optimisation approach (Figure 2). That means, from a set of parameters (decision variables) cycles are generated and integrated into the process, than evaluated regarding multiple objectives. The best ones are kept in order to create a list of Pareto-optimal solutions. The distinctive feature of our approach from similar analyses like (Wang, 2013) is the resolution of the integration (slave-problem of the multi objective optimisation) is done at the same time for all fluids that are available in the used thermodynamic solution engine.

2.1 Objectives

In order to identify which cycles should be used within a particular industrial setting, one has to be clear about the objectives on which the choice is based. Objectives from different areas are thinkable, thermodynamic performance, economic indicators, environmental objectives etc. A trade-off between different objectives can be represented by a list of Pareto-optimal solutions, where no objective can be increased without decreasing another. The final choice or the weight between the objectives depends on the responsible persons for a possible investment.
For this paper we will consider two types of objectives:

- Cost minimisation
- Exergy Efficiency maximisation

The objectives are calculated by the use of a post-computation, after the integration.

2.2 Parameters and Constraints

There are several parameters that have to be set or chosen. Some parameters are set up front in order to meet requirements and others will be used as decision variables for the identification of the Pareto-optimal solutions. There are qualitative and quantitative parameters that can be constrained before starting the optimisation. Examples for qualitative parameters are characteristics of the fluids like toxicity or flammability, quantitative parameter are for example thermodynamic parameters like pressure or temperature limits. Here we will constrain the example problem and chose a maximum Global Warming Potential (GWP) and Ozone Depletion Potential (ODP) of the working fluids considered, up front.
As an important design parameter, the number of stages and cycles can be forced to a certain number or to be larger or smaller than a certain number.
In order to minimize the decision variables, the sub-cooling temperature difference is fixed as well as the mass flow rate of the cycle. The final mass flow rate and thus the size of the cycle will of course be adapted in the process integration step; this means that depending on the initial size chosen, the solver of the integration step has to find a multiplication factor. In our experience, choosing a base size within one or two orders of magnitude of the final solution facilitates the quick convergence of the solver.
The choice of fluids is limited to the REFPROP data base (Lemmon et al., 2010) which we use for all thermodynamic calculations in order to get coherent results.
Other parameters that are fixed are turbine and pump isentropic efficiencies.
The decision variables used for the optimisation in this paper:

- Turbine inlet temperature
- Turbine inlet/Evaporation Pressure
- Minimum Temperature Difference (DT_{min}) in heat exchanges
- Condensation start Temperature

These parameters allow for fitting with differently shaped heat sources and heat sinks. Also they allow for maximum flexibility in the choice of the cycle, since they can be applied as well for classical organic Rankine cycles as well as for mixtures or supercritical cycles.

2.3 Genetic Algorithm

In order to generate the list of Pareto-optimal solutions a genetic algorithm is used; it acts as an optimiser for the Multi Objective Optimisation (MOO). This algorithm is designed to copy the behaviour of an accelerated evolution. At first a number of random sets of decision variables, representing the gens, is created and the resulting cycles (individuals of initial population) are calculated. Afterwards the gens/decision variables can be combined from two individuals and/or mutated. The algorithm keeps the individuals that behave well regarding the objectives and converges thus towards the Pareto-curve (set of Pareto-optimal solutions). The concept is developed in (Kemp, 2007) and has been widely applied, e.g. in (Klemeš, 2013). The advantage of this optimising algorithm is that the physical models can be developed entirely separated, meaning also in separate software, and no equations have to be passed on to the optimiser, only the results. This makes it extremely versatile and makes it especially suitable for non-continuous problems.

2.4 Thermodynamic Models I

The first thermodynamic models are used to calculate the states of the working fluid and the mechanical and thermal streams into and out of the cycles. REFPROP database and equations are used to this end. The sequence of calculations is to check the feasibility and calculate the characteristics of the cycles with the generated decision variables. All feasible cycles are then calculated entirely and the corresponding streams defined, they are put to the test in the MILP-Solver (described below in chapter 2.7).

2.5 Thermodynamic Models II

The second set of thermodynamic models is used to calculate heat transfer coefficients and with those the resulting heat exchanger surfaces. The surfaces are needed for economic evaluations since the quantity of heat exchanged and the Pinch temperature in a heat exchanger represent a trade-off with the investment cost.

The interest of this methodology is to identify and qualify relative behaviour of working fluids; we thus consider only one model heat exchanger for all the fluids in order to calculate the heat transfer coefficients. This is not supposed to be the design of a finally used heat exchanger, but to make a ranking between the fluids possible.

The heat exchange surface calculation is done before the integration of the cycle into the process; it is for this reason impossible to obtain the final surface, which would require the final temperatures between heat sources and sinks. The temperature difference between sinks and sources is therefore assumed to be equal to DT_{min} at every point. Thus, the estimation is conservative and less integrated solutions (with big temperature differences between cycle and process streams) are penalised in regard to well integrated (small temperature differences, close to DT_{min}) solutions.

The heat transfer coefficient cannot be calculated the same way for every point, the methods used here are:

Dittus-Boelter-Equation (Incropera et al., 2011) used for: Pre-heating; Super-heating; De-super-heating; Sub-cooling; Entire heating for Super-/Trans-Critical-Cycles):

$$\mathrm{Nu} = 0.23\mathrm{Re}^{0.8}\mathrm{Pr}^{n} \tag{1}$$

Where n=0.4 for heating and 0.3 for cooling.

The VDI-Method Hbb (VDI, 2006) (supposed vertical tubes) is used for evaporation:

$$\frac{\alpha(z)_k}{\alpha_{LO}} = \left\{(1-\dot{x})^{0.01}\left[(1-\dot{x})^{1.5} + 1.9\dot{x}^{0.6}\left(\frac{\rho'}{\rho''}\right)^{0.35}\right]^{-2.2} + \dot{x}^{0.6}\left[\frac{\alpha_{GO}}{\alpha_{LO}}\left(1 + 8(1-\dot{x})^{0.7}\left(\frac{\rho'}{\rho''}\right)^{0.67}\right)\right]^{-2}\right\}^{-0.5} \tag{2}$$

LO – entire mass flow liquid; GO – entire mass flow gaseous; $\dot{x}$ – fraction of vapour flow

The VDI-Method Ja (VDI, 2006) (supposed vertical tubes) is used for condensation):

$$\mathrm{Nu}_{\mathrm{F,x}}^{*} = \sqrt{\left(\mathrm{K}_{\mathrm{Ph,l}}\mathrm{Nu}_{\mathrm{F,x,l}}\right)^{2} + \left(\mathrm{K}_{\mathrm{Ph,t}}\mathrm{Nu}_{\mathrm{F,x,t}}\right)^{2}} \quad (3)$$

With t for turbulent, l for laminar and K_{Ph} the correction factor for phase limit. An average value over $\dot{x}$ is calculated and used for the last two methods.

2.6 Economic Models

The MILP solver responsible for the integration can be used for optimising different characteristics. If a cost optimisation is selected for the integration, the solver the possibility to choose between different solutions: The use (integer) and the size of the proposed cycles (linear multiplication factor) are set in this step. The differences between fluids are made quantifiable by producing grass root costs using the cost functions defined by Turton (2012). The cost functions of Turton have to be linearized for the MILP-solver to a form *c*=*a*+*bx* where *x* is the multiplication factor, describing the impact of the size on the cost and *a* is the base cost, independent of size.

The correlation of the linearization with the original cost functions is very good since the applicable range has been chosen relatively narrow. Exceeding the linearized area will lead to an overestimation of pump (31 % if exceeded 5 times) and expander cost (66 % if exceeded 5 times), and an underestimation of the heat exchanger cost (15 % if the heat exchange area is exceeded 5 times).Overall cost will be overestimated for larger installations. If the range of the system should be different, the cost calculations should be adapted. The linearization of the three considered units is shown in the following figures (Figures 3 to 5).

With the above, the investment cost can be calculated and from there the grass root cost, accounting for annualisation, material and pressure as well as bare modul factor, following (Turton, 2012). Thereafter, the operation cost has to be added. Like in the publication (Lazzaretto, 2011) two per cent of the Investment cost is assumed to occur as operation cost during the lifetime of the system. Lifetime is assumed to be 15 y and yearly operating time 8,000 h. Since the markets for electricity and other energy sources have shown to be volatile and unpredictable during the last years, the prices (electricity and operation cost) are simply assumed to develop with the value of money, so no depreciation term has to be included. Heat recovery is mostly interesting for larger industrial sites, so the entire electricity is assumed to replace electricity import/purchase thus the price is based on the purchasing price taken from Eurostat 2012 (Eurostat, 2013) second semester for industry with 2,000 to 20,000 MWh Band. The net shaft power includes turbine and pump shaft power.

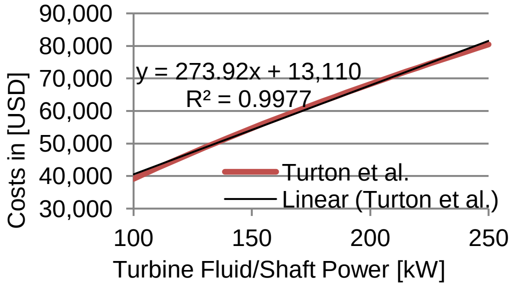

Figure 3: Linearization of cost function – Turbine

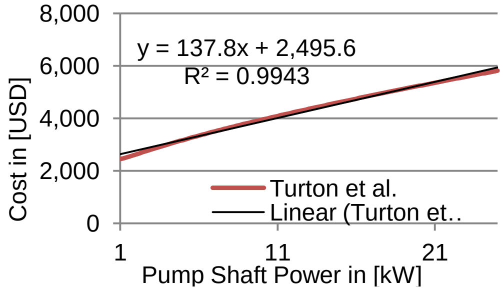

Figure 4: Linearization of cost function – Pump

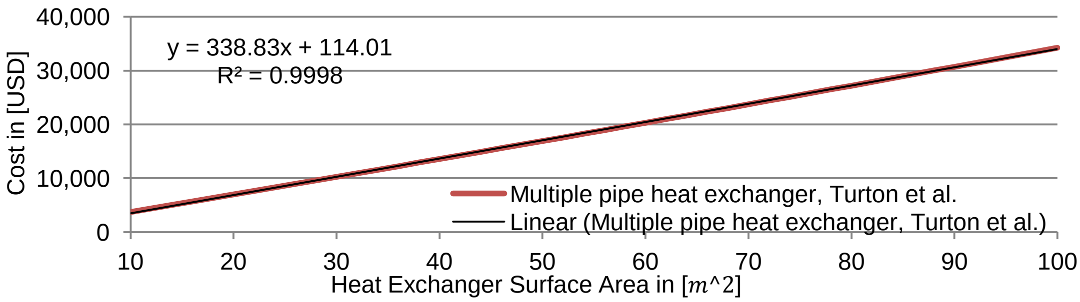

Figure 5: Linearization of cost function – Heat Exchangers

Four values are calculated Cost1 and 2 describing the operating cost, Cinv1 and 2 describing the Grass root cost, the first values Cost1 and Cinv1 correspond to the size independent part a.

- $\mathrm{Cost1} = 0.02 * (\text{fix part of GrassRootInvestments})$
- $\mathrm{Cost2} =$
  $-\frac{8{,}000\ \mathrm{h}}{\mathrm{y}} * 15\ \mathrm{y} * \frac{0.1574\ \mathrm{EUR}}{\mathrm{kWh}} * \frac{1.32\ \mathrm{USD}}{\mathrm{EUR}} * (\text{net Shaft Power}) + 0.02 *$
  $(\text{size depending part of GrassRootInvestments})$
- $\mathrm{Cinv1} = \text{fix part of GrassRootInvestment}$
- $\mathrm{Cinv2} = \text{size depending part of GrassRootInvestment}$

The costs calculated this way are not to be understood as final cost estimations of the installation. As mentioned above the temperature differences in the heat exchanger do not correspond to the final temperature differences, thus overestimating the cost of them. The costs are however used in order to rank the different options and will be normalised between zero and one in order to make an educated choice of a fluid.

2.7 Integration – MILP-Solver

The integration uses the tools of pinch analysis and is done by a Mixed Integer Linear Programming (MILP) solver. An MILP problem is a problem that contains at the same time linear equations (including equalities, maximisations and minimisations) as well as integer problems (these can be on-off problems, e.g. shall a unit be used or not, or negative and positive whole number problems for example for the number of stages in a cycle). The solver is used to resolve a mathematical problem containing linear equations and integer values. Here we use a solver by IBM called ILOG CPLEX. The linear equations are the heat cascade and the sizing of the cycles as well as the objective functions and the cost functions.

Every possible cycle for the analysed set of decision variables is thus fitted into the process, this makes sizing necessary, a sizing parameter (multiplication factor of the predefined size) is applied, this is done for the thermodynamic characteristics (energy balances) and also for the cost parameters (size depending parts).

The integer problems give the possibility to use or not use a proposed cycle. An additional constraint is imposed which decides on minimum, maximum or specific numbers of cycles to be integrated with the process. If more than one cycle is allowed, it is logical to increase the number of decision variables such (multiply by the number of units), thus several cycles with independent characteristics (pressure levels, temperatures etc) can be combined.

The MILP-Solver solves the problem for all cycles corresponding to the set of decision variables at once. This way it is choosing between all fluids from the REFPROP database that comply with the choices made in the beginning (ODP, GDP etc) and are feasible.

In order to make the decision, one objective has to be chosen for the solver, it can either be thermodynamic (maximizing the power output) or financial (minimizing the total cost/maximizing the benefits). The resulting cycle (or cycles) that are than send back to the Multi Objective Optimiser, depends on the chosen objective and a careful choice on the objective has to be done. The resolution time depends strongly on the number of integer variables.

2.8 Post-Calculation – Indicators

In a post-calculation, the objectives are calculated based on the results of the MILP-solution. Different indicators can be calculated, these can then be used as objectives for the Multi Objective Optimisation and as additional information for further evaluation. If an indicator is used as an objective in the MOO it is sent to the genetic algorithm and used for the further evolution of the new individual, compared to the existing population.

3. Application Example

To illustrate the methodology an example is chosen, taken from an industrial process (clinker production) that presents two heat sources and that is already coupled with a district heating process. The constraints were a pressure in the range of 0.1 to 50 bar and a global warming potential (GWP) lower or equal to that of r-245fa (1030), furthermore all fluids with a flammability of “3” and/or toxicity of “A” following the ASHRAE (Ashrae, 2013) classification have been excluded and two cycles or one two stage cycles were admitted. Below can be seen the Pareto front (Figure 6) and the integrated composite curve in a Carnot-factor over heat load diagram (Figure 7) of one Pareto optimal point (flash).

4. Conclusions

We present a methodology that is adequate for the identification of suitable working fluids and cycles for electricity production. Using a multi objective optimisation (MOO) as a master-problem and the integration

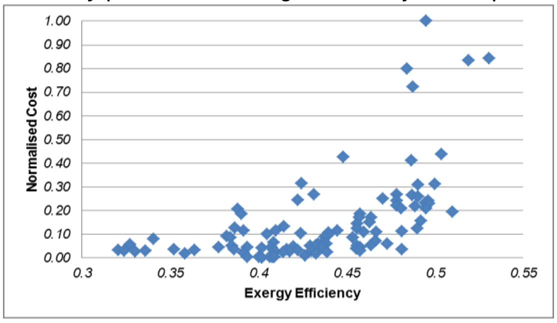

Figure 6: Pareto-Front of cycles

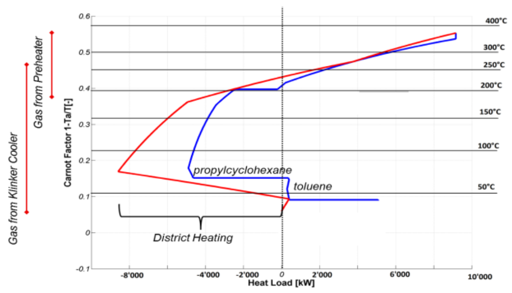

Figure 7: Integrated Composite Curves example cycles

of the cycle(s) with the process, as well as the choice of the working fluid(s) with the MILP-solver as a slave problem ensures that all possible fluids are tested the best choice for the set of decision variables is made. This reduces the problem greatly since the fluid selection is not a decision variable. Using the cost aspect is a way to account for differences in heat transfer and the electricity production at the same time. Further development can be done, regarding estimation of final cost in a post calculation for the MOO and regarding mixtures, since here only predefined mixtures of the REFPROP database are included.

References

ASHRAE., 2013. ASHRAE Handbook of Fundamentals, ASHRAE.

Bendig M., Maréchal F., Favrat D., 2012. Defining the potential of usable waste heat in industrial processes with the help of pinch and exergy analysis. Chemical Eng Transactions, 29, 103–108.

Bendig M., Maréchal F., Favrat D., 2013. Defining “Waste Heat” for industrial processes. Applied Thermal Engineering, 61(1), S.134–142.

Borel L., Favrat, D., 2010. Thermodynamics and Energetics for Engineers, EPFL Press.

Eurostat, 2013, Electricity prices charged to industrial consumers, <appsso.eurostat.ec.europa.eu/nui/submitViewTableAction.do> accessed 05.12.2013.

Heberle F., Preißinger M., Brüggemann D., 2012. Zeotropic mixtures as working fluids in Organic Rankine Cycles for low-enthalpy geothermal resources. Renewable Energy, 37(1), S.364–370.

Incropera F.P., Lavine A.S., DeWitt D.P., 2011. Fundamentals of Heat and Mass Transfer, John Wiley & Sons, New York, USA.

Kemp I.C., 2007. Pinch analysis and process integration: a user guide on process integration for the efficient use of energy, Butterworth-Heinemann, Oxford, UK.

Klemeš J.(ed), 2013. Handbook of Process Integration (PI), Cambridge: Woodhead Publishing/Elsevier, UK.

Lazzaretto A., Toffolo A., Manente G., Rossi N., Paci M., 2011. Cost evaluation of organic Rankine cycles for low temperature geothermal sources. Proceedings 24th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, 3854–3868, Serbia.

Maraver D., Uche J., Royo J., 2012. Assessment of high temperature organic Rankine cycle engine for polygeneration with MED desalination: A preliminary approach. Engy Conv and Man 53(1), S.108–117.

Lemmon E., Huber M., McLinden M., 2010. NIST Standard ReferenceDatabase 23: Reference Fluid Thermodynamic and Transport Properties - REFPROP. 9.0. <nist.gov/srd/nist23.cfm> accessed 14.02.2014.

Schuster, A., Karellas, S., Kakaras, E., Spliethoff, H., 2009. Energetic and economic investigation of Organic Rankine Cycle applications. Applied Thermal Engineering, 29(8-9), S.1809–1817.

Turton R., 2012. Analysis, synthesis, and design of chemical processes, Upper Saddle River, N.J: Pearson, USA..

Verein Deutscher Ingenieure (VDI), 2006. Calculation of Heat Exchangers). In VDI-Wärmeatlas. VDI Buch. Springer Berlin Heidelberg, Germany. (in German)

Wang, J., Yan, Z., Wang, M., Li, M., Dai, Y.,, 2013. Multi-objective optimization of an organic Rankine cycle (ORC) for low grade waste heat recovery using evolutionary algorithm. Energy Conversion and Management, 71, S.146–158.