Dynamic simulation and optimisation of water and energy consumption in a ceramic plant: Application of the customised ThermWatt computational tool

Miguel Castro Oliveira a,b, Rita Castro Oliveira c, Henrique A. Matos b

a Low Carbon & Resource Efficiency, R&Di, Instituto de Soldadura e Qualidade, 2740-120 Porto Salvo, Portugal

b Department of Chemical Engineering, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049-001 Lisboa, Portugal

c Department of Computer Science and Engineering, Instituto Superior Técnico, Universidade de Lisboa, Avenida Rovisco Pais 1, 1049-001 Lisboa, Portugal

Abstract

In this work, complex models developed for the project of Water and Energy Integration Systems (WEIS) in a ceramic industry plant are presented. The WEIS is an innovative concept of systems that consider the recirculation of water and energy streams in a plant to produce overall water and energy efficiency improvement-related benefits. These models have been created in the scope of the development of a computational tool and derivate Engineering service designated as ThermWatt (using both the Modelica and Python languages). A post-processing assessment to the results of the final simulation model allowed the estimation of 2 years and 10 months payback time and a reduction of 1.76 kton CO2,eq/ year, which are highly favourable results compared to the benchmarks defined for the European.

**Keywords**: Water and energy integration systems, water-energy nexus, thermal energy storage, Python NLP-model, Modelica DP-model.

* 1. Introduction

The whole production process in manufacturing plants requires the use of significant quantities of natural resources, with water and energy being two of the most relevant categories of these resources (Walsh et al., 2015). The recirculation of resources, for instance, through waste heat recovery and water recirculation, constitutes a set of measures that may solve the issues related to the overuse of resources. One of the challenges related to such measures’ implementation is the existence of intermittent operations.

Most recently, researchers have proposed the implementation of new conceptual systems designated as Water and Energy Integration Systems (WEIS), which contemplate water and waste heat stream recirculation (Castro Oliveira et al., 2022). These studies have been supported by the use of simulation and optimisation models, namely with a customised tool named ThermWatt (Castro Oliveira et al., 2022a, 2023). Although these systems have been proved to be successful in the fulfilment of the aims related to water and energy use reduction and all the economic and environmental benefits thereof, the WEIS have only been conceptualized and analysed in a steady-state based perspective, not considering a transient-based perspective, such as with the presence of intermittent combustion-based processes and the installation of thermal energy storage (TES) units.

In this work, a set of computational models using the overall capabilities of the ThermWatt tool are developed for a WEIS set to be installed in a ceramic plant, in which TES are conceptually set to be installed to reduce the energy use in intermittent combustion-based processes. The goal of this work is to obtain a final dynamic simulation model, to achieve water and energy use reduction-related economic and environmental benefits.

* 1. Characterization of the Case-study

The case-study is set in a sanitaryware plant installed in Portugal, containing three water-using lines (three water-using processes, three heaters and three coolers), two tunnel kilns (continuous combustion-based processes) and two intermittent kilns (intermittent combustion-based processes). All the combustion-based processes use natural gas as fuel. The water-using processes make use of a water stream to remove determinate quantities of three non-identified salts (designated by the indexes 1, 2 and 3). Each outlet wastewater (saline water) stream is associated to determinate minimum and maximum concentrations for each salt. The baseline scenario of the plant encompassing the identified processes is characterized in the sequence of Figures 1 and 2.



**Figure 1.** Flowsheets of the water-using lines

****

**Figure 2.** Flowsheets of combustion-based processes: Kilns a) 1, b) 2, c) 3, d) 4

The conceptualized WEIS for the approached case-study may be characterized by the following sequence of steps:

* The superstructure configuration considers the processes presented in Figures 1 and 2 as baseline, in addition to several recirculation points and technologies, as described in the points below;
* Each one of the two tunnel is characterized by having two waste heat streams: exhaust gas streams and hot air streams;
* An Organic Rankine cycle (ORC) is considered for electricity generation from enthalpy withdrawal from a mixed gas (hot air and exhaust gas mixture) stream;
* A MED unit is considered as the wastewater treatment unit (treatment of the saline water stream at the outlet of the water-using processes);
* An Electrolysis unit is considered for the generation of green hydrogen from the discharge water stream from the water system;
* The hydrogen produced in the Electrolysis unit is distributed to the fuel inlet of each one of the tunnel kilns so to produce hydrogen-enriched natural gas (HENG);
* A PCM-based heat exchanger is used for enthalpy withdrawal from a mixture of part of the hot air from both tunnel kilns (during the cooling phase of the intermittent kilns, which is enthalpy charge phase to the TES unit) and to supply additional enthalpy to the ambient air streams at the inlet of each one of the combustion-based processes kilns (during the firing phase of the intermittent kilns, which is enthalpy discharge phase to the TES unit);
* During the cooling cycle of the kilns, the respective part of the mixture hot air streams from each one of the tunnel kilns is recirculated to the ORC
* The hot air streams from each one of the two tunnel kilns are recirculated to the respective tunnel kiln and to the HRSG unit of the ORC;
* The remaining quantities of the hot air streams from each one of the two tunnel kilns are mixed and recirculated to three water-gas heat exchangers (economisers) installed to heat up the inlet water stream at each one of the water system’s heaters and the first effect of the MED unit;
* The hot air streams at the outlet of the water-gas heat exchangers and the MED unit are then conjoined and furtherly recirculated to be mixed with the conjoined exhaust gas streams, so then the mixed gas stream to be recirculated to the ORC.
	1. Simulation and Optimisation Models

A complex modelling framework has been developed in the scope of this work. A total of three models have been created: a non-linear programming (NLP) model for the water system developed in Python, a dynamic programming (DP) model developed for the thermal process system in Modelica and a final dynamic simulation model (which integrates the results of the two optimisation models) also developed in Modelica. Since the final simulation model is the ultimate end of the work in terms of modelling, the numerical results obtained by the two counterpart optimisation models had to be allocated to the final model. For the water system NLP model, the results may be allocated from the Python-NLP model to the Modelica model using the OpenModelica Python API. However, a similar API does not exist for the allocation of results between the two Modelica models, and it is impossible to run the two models within the same script due to need of different solvers for each one (*optimization* solver for the DP model and DASSL for the final model). Although that is not considered an issue in respect to the objectives of the work, which are based on the obtention of water and energy use-related benefits, such may be a challenge to be attended in further developments of the ThermWatt tool. In the sequence of these, Tables 1 and 2 shows the model characterization with only the equality constraints of interest, with thew whole set of equations characterizing a WEIS (including trivial ones) have already delineated for a similar case-study in a previous work (Castro Oliveira et al., 2023). The considered inequality constraints are only defined as the lower and upper limit values for variables, as defined in Figures 1 and 2. In Figure 3, the final simulation model is presented, in the form of the flowsheet of the optimal WEIS configuration (considering the values of the parameters characterizing each stream of interest and only the streams and technologies making part of the final optimal scenario, and not the whole superstructure). In relation to the constant values presented in Tables 1 and 2, is to note:

* ${1}/{4}$ refers to the splitting of the water stream from the MED unit condenser to each one of the four effects;
* $418.896$ (with kJ/kg units) refers to the specific enthalpy of saturated liquid water;
* $2675.43$ (with kJ/kg units) refers to the specific enthalpy of saturated steam;
* $999$ (with kg/ m3 units) refers to the density of liquid water.
* $0.0422$ refers to the thermal-to-electric conversion efficiency associated to the ORC;
* $3600$ (with kJ/kWh units) refers to the factor of conversion of kWh to kJ energy units;
* $0.15$ (with W/(m.ºC) units) refers to the thermal conductivity of the considered PCM;
* $890$ (with kg/m3 units) refers to the density of the considered PCM;
* $225000$ (with J/kg units) refers to the latent enthalpy associated to the melting/ solidification of PCM (as required as a parameter on the apparent specific heat capacity determination equation);
* $3.1416$ is an approximation of pi;
* $0.1626$ (with ºC units) refers to the temperature constant for the PCM microstructure;
* $72$ (with ºC units) refers to lower bound for the temperature range of phase change of the PCM;
* $2200$ (with J/(ºC.kg) units) refers to the specific heat capacity for the solid phase of the PCM.

**Table 1.** Characterization of the non-linear programming (NLP) model

|  |
| --- |
| **Decision Variables** |
| * Freshwater mass flow rate ($\dot{M}\_{FW}$)
* Each water stream mass flow rate ($\dot{M}\_{W}$)
* Each water stream specific enthalpy ($h\_{W}$)/ temperature ($T\_{W}$)
 | * Each water stream contaminant concentration ($C\_{W}$)
* Consumption of hot utilities ($q\_{Hot.Ut.}$) and cold utilities ($q\_{Cold.Ut.}$)
* Heat transfer area of economisers ($A\_{Econ.}$)
* Heat transfer area of MED Effect 1 ($A\_{Eff1}$)
 |
| **Equality Constraints** |
| $$\dot{M}\_{W.,in,Eff}·{1}/{4}=\dot{M}\_{TW.,Eff}+\dot{M}\_{Concentrate,Eff}$$ | (1) |
| $$q\_{with.,MED}-\dot{M}\_{TW.,Eff1}·\left(h\_{V,Eff1}-418.896\right)=\dot{M}\_{W.,in,Eff1}·{1}/{4}·\left(418.896-h\_{w,in,Eff}\right)$$ | (2) |
| $$\dot{M}\_{TW.,Eff k-1}·\left(h\_{V,Eff1}-418.896\right)=\dot{M}\_{TW.,Effk}·\left(h\_{V,Effk}-418.896\right)+\dot{M}\_{W.,in,Effk}·{1}/{4}·\left(418.896-h\_{w,in,Eff}\right)$$ | (3) |
| $$\dot{M}\_{TW.,Effect}·\left(2675.43 -418.896\right)=\dot{M}\_{W.,in,Eff}·{1}/{4}·\left(h\_{Vapour,Eff1}-418.896\right)$$ | (4) |
| $$q\_{with.}=U·A·\left(\left(T\_{Air,in}-T\_{w,out}\right)·\left(T\_{Air,out}-T\_{w,in}\right)·\left(\left(T\_{Air,in}-T\_{w,out}\right)+\left(T\_{Air,out}-T\_{w,in}\right)\right)·0.5\right)^{{1}/{3}}$$ | (5) |
| **Objective-Function** (Unitary water and energy prices for Portugal) |
| $$min\left(1.8499\left(€/m^{3}\right)·{1}/{999}\left(m^{3}/kg\right)·\dot{M}\_{FW}\left(kg/h\right)+23.66\left(€/GJ\right)·q\_{Hot.Ut.}\left(GJ/h\right)+0.1459\left(€/kWh\right)·{1}/{0.95}·{1}/{3600}\left(kWh/GJ\right)·q\_{Cold.Ut.}\left(GJ/h\right)\right)\left(€/h\right)$$ | (6) |

**Table 2.** Characterization of the dynamic programming (DP) model

|  |
| --- |
| **Decision Variables** |
| * Natural gas flow rates ($\dot{M}\_{Fuel}$)
* Ambient air flow rates ($\dot{M}\_{Amb. Air}$)
* Exhaust gases flow rates ($\dot{M}\_{Ex.}$)
* Exhaust gases specific enthalpies ($h\_{Ex.}$)
* Hot air flow rates ($\dot{M}\_{Hot Air}$)
* Hot air specific enthalpies ($h\_{Hot Air}$)/ temperatures ($T\_{Hot Air}$)
 | * Recirculated air flow rates ($\dot{M}\_{Rec. Air}$)
* Recirculated air specific enthalpies ($h\_{Rec Air}$) and temperatures ($T\_{Rec Air}$)
* Generated electricity ($Elec\_{Eff}$)
* Thermal storage material temperature ($T\_{PCM}$)
* Thermal storage material apparent specific heat capacity ($C\_{PCM}$)
* External ($r\_{ext}$) and internal radius ($r\_{int}$) of the TES unit
 |
| **Relevant Start Values** |
| Temperature of the PCM within the TES unit ($T\_{PCM}$) (ºC) | 41.5 |
| **Equality Constraints** |
| Thermal Process System (Stream Recirculation) |
| $$\dot{M}\_{Comb. Air}=\dot{M}\_{Rec.Air}+\dot{M}\_{Amb. Air}$$ | (7) |
| $$\dot{M}\_{C. Air}·h\_{Comb. Air}=\dot{M}\_{Rec.Air}·h\_{Recyc. Air}+\dot{M}\_{Amb. Air}·h\_{Amb. Air}$$ | (8) |
| $$\dot{M}\_{Fuel}+\dot{M}\_{C. Air}=\dot{M}\_{Ex.}$$ | (9) |
| $$\dot{M}\_{Fuel}·AF=\dot{M}\_{C. Air}$$ | (10) |
| $$\dot{M}\_{gas,in,ORC}·\left(h\_{gas,in,ORC}-h\_{gas,out,ORC}\right)·0.0422=Elec∙3600$$ | (11) |
| Thermal Energy Storage-Related |
| Charge Phase | $$\frac{dT\_{PCM}}{dt}=\frac{0.15}{890·C\_{PCM}}·\frac{1}{\left(r\_{ext}+r\_{int}\right)·0.5}·\left(\left(\frac{T\_{PCM,N}-T\_{PCM,1}}{r\_{ext}-r\_{int}}\right)+\left(\frac{T\_{PCM,N}-2·T\_{PCM}+T\_{PCM,1}}{\left(r\_{ext}-r\_{int}\right)^{2}}\right)\right)$$ | (12) |
| Discharge Phase | $$\frac{dT\_{PCM}}{dt}=\frac{0.15}{890·C\_{PCM}}·\frac{1}{\left(r\_{ext}+r\_{int}\right)·0.5}·\left(\left(\frac{T\_{PCM,1}-T\_{PCM,N}}{r\_{ext}-r\_{int}}\right)+\left(\frac{T\_{PCM,1}-2·T\_{PCM}+T\_{PCM,N}}{\left(r\_{ext}-r\_{int}\right)^{2}}\right)\right)$$ | (13) |
| $$C\_{PCM}=\frac{225000}{\left(2·3.1416\right)^{0.5}·0.1626}·exp\left(\frac{-\left(T\_{PCM}-72\right)^{2}}{2·0.1626^{2}}\right)+2200$$ | (14) |
| **Objective-Function** (Unitary water and energy prices for Portugal) |
| $$OBJ=\left(\left(23.66\left(€/GJ\right)·0.0453\left(GJ/kg\right)·\dot{M}\_{Fuel}\left(kg/h\right)-0.1459\left(€/kWh\right)·Elec\_{Eff}\left(kWh/h\right)\right)·{1}/{3600}\left(s/h\right)\right)\left(€/s\right)$$ | (15) |
| $$OBJ\left(€/s\right)=\left(\frac{d}{dt}\left(OBJEff\left(€\right)\right)\right)\left(€/s\right)$$ | (16) |
| $$min\left(OBJEff \left(t=151200 s\right) \left(€\right)\right), OBJEff \left(t=0 s\right)=0 €$$ | (17) |

|  |
| --- |
| **Figure 3.** Flowsheet assembling of the Final Configuration using the ThermWatt Modelica library capabilities (darker colour: corresponding values to the optimisation model, lighter colour: referent to variables that are only part of the simulation model) |

* 1. Post-processing – Economic and Environmental Impact Assessment

The obtained results for stream allocation must be analysed at the light of economic and environmental impact reduction-related benefits. In Table 3, the results for economic and environmental impact assessment are presented.

**Table 3.** Economic and Environmental Impact Reduction Assessments

|  |
| --- |
| **Natural gas consumption (kg/cycle)** |
| **Process** | **Initial** | **Improved** | **Relative Savings Share** | **Savings (€/cycle)** |
| **Kiln 1** | 5355.00 | 4530.38 | 15.40% | 879.92 |
| **Kiln 2** | 5044.20 | 3529.69 | 30.02% | 1616.08 |
| **Kiln 3** | 334.29 | 318.18 | 4.82% | 17.19 |
| **Kiln 4** | 1266.05 | 1230.65 | 2.80% | 37.78 |
| **Hot and Cold utilities consumption (GJ/h)** |
| **Process** | **Initial** | **Improved** | **Relative Savings Share** | **Savings (€/h)** |
| **Heaters (3)** | 0.338 |  | 100.00% | 7.998 |
| **Coolers (3)** | 0.235 |  | 100.00% | 9.502 |
| **Water consumption (m3/h)** |
| **Initial** | **Improved** | **Relative Savings Share** | **Savings (€/h)** |
| 0.861 | 0.529 | 38.57% | 0.61 |
| **Electricity Balances (kWh/h)** |
| **Net Electricity Generation (kWh/h)** | **Savings (€/h)** |
| 771.89 | 112.62 |
| **Final assessment** |
| **Energy Savings** | **CAPEX (k€)** | **Savings (k€/year)** | **Payback Time (Years)** | $CO\_{2,eq}$ **emissions reduction (****kton/year)** |
| 6.88% | 1802.81 | 637.91 | 2.83 | 1.76 |

The results are highly favourable compared to industrial benchmarks defined for the European industry (2 – 3 years payback time and 0.775 kton CO2,eq/ year reduction).

* 1. Conclusions

This work approaches the assessment of potential improvements of the overall water and energy efficiencies in a ceramic industry plant through the development and further use of a complex modelling framework (encompassing a set of simulation and optimisation models), as part of a customised tool designated as ThermWatt. The models were developed with the aim to apply the newly created methodology of Water and Energy Integration Systems (WEIS). The developed models proved to be valuable for the achievement of the proposed objectives. A set of indicators were assessed in post-processing, having been obtained a payback period of about of 2 years and 10 months and an emission reduction level of 1.76 kton CO2,eq/year, which are highly favourable compared to industrial benchmarks defined for the European industry, associated to 6.88% overall energy savings and 38.57% water savings.

Acknowledgements

This work and conference participation was funded through the base funding component of the Center for Technology and Innovation – ISQ, under the terms defined in AAC nº 03/C05-i02/2022, and CERENA under grant UIDB/04028/2020\_UIDP/04028/2020.

References

M. Castro Oliveira, M. Iten, H.A. Matos, 2023, Simultaneous optimisation of energy recovery and water recirculation in a ceramic plant. Comput. Aided Chem. Eng. 52, 2785–2790.

M. Castro Oliveira, M. Iten, H.A. Matos, 2022, Simulation and assessment of an integrated thermal processes and Organic Rankine Cycle (ORC) system with Modelica. Energy Reports 8, 764–770.

M. Castro Oliveira, M. Iten, H.A. Matos, 2022a, Review on Water and Energy Integration in Process Industry: Water-Heat Nexus. Sustain. 14.

B.P. Walsh, S.N. Murray, D.T.J. O’Sullivan, 2015. The water energy nexus, an ISO50001 water case study and the need for a water value system. Water Resour. Ind. 10, 15–28.