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Methodology to assess the integrity of Water and Energy Integration Systems (WEIS) models using the ThermWatt computational tool

Miguel Castro Oliveira[a,b]*, Rita Castro Oliveira[c] and Henrique A. Matos[b]

[a] Research, Development and Innovation, Instituto de Soldadura e Qualidade, 2740-120 Porto Salvo, Portugal
[b] Centro de Recursos Naturais e Ambiente (CERENA), Department of Chemical Engineering, Instituto Superior Técnico, Avenida Rovisco Pais 1, 1049-001 Lisboa, Portugal
[c] Department of Computer Science and Engineering, Instituto Superior Técnico, Avenida Rovisco Pais 1, 1049-001 Lisboa, Portugal
* Corresponding Author: dmoliveira@isq.pt, miguelmcoliveira@tecnico.ulisboa.pt.

ABSTRACT

Type your abstract text here. This work presents an essential methodological framework oriented to the implementation of sustainability promotion measures in process industries. It makes use of a previously developed paradigm, designated as Water and Energy Integration Systems (WEIS), which are fundamentally conceptual systems based on the implementation of several technologies implemented with the end to minimize water use, energy use and related environmental burdens. The primarily conceptual nature of these systems is significant that these have not been significantly implemented in real-life, and that these have been essentially implemented in the virtual basis of digital twin-based computational models. This work extensively presents a methodology developed for the assessment of the integrity of WEIS models, which have been developed using the capacities of a customised computational tool designated as ThermWatt. Two previously approached case-studies have been considered to perform a proof-of-concept in respect to the applicability of the delineated methodology. The delineated methodology proved to be adequate for the whole process of the elaboration of the WEIS Engineering projects, paving way to the implementation of these in real-life in a future perspective.

Keywords: Water and energy integration systems, simulation, optimisation, model integrity, sustainability promotion

INTRODUCTION

This is Header 2Water and Energy Integration Systems (WEIS) subsist in complex installations to be installed in end-use sector facilities set to perform the maximum use of the recirculation of waste heat and water streams for the purpose of causing an overall sustainability promotion. These systems use a set of technologies that may be used in the context of the exploitation of the interdependencies of energy and water resources, as encompassed by the concept of water-energy nexus [1].

The WEIS paradigm was introduced and extensively developed in previous works developed by the authors [2], along with the tool created for the purpose of modelling, the ThermWatt computational tool [3]. This tool subsists in several simulation and optimisation models created in the Modelica and Python languages, which fundamentally serve as digital twins of real-life installations.

The duality between the WEIS paradigm and the ThermWatt tool has been making possible the existence of a complex framework in which the viability associated to sustainability promotion technologies-based systems is set to be firstly assessed in a virtual basis. In this sense, it is possible to develop proposals of systems that promote overall sustainability in a site with minimized requirements of real-life testing of technologies to be implemented. Owing to the primarily conceptual nature of the WEIS paradigm, the assurance of the integrity of computational models of this type of systems is essential

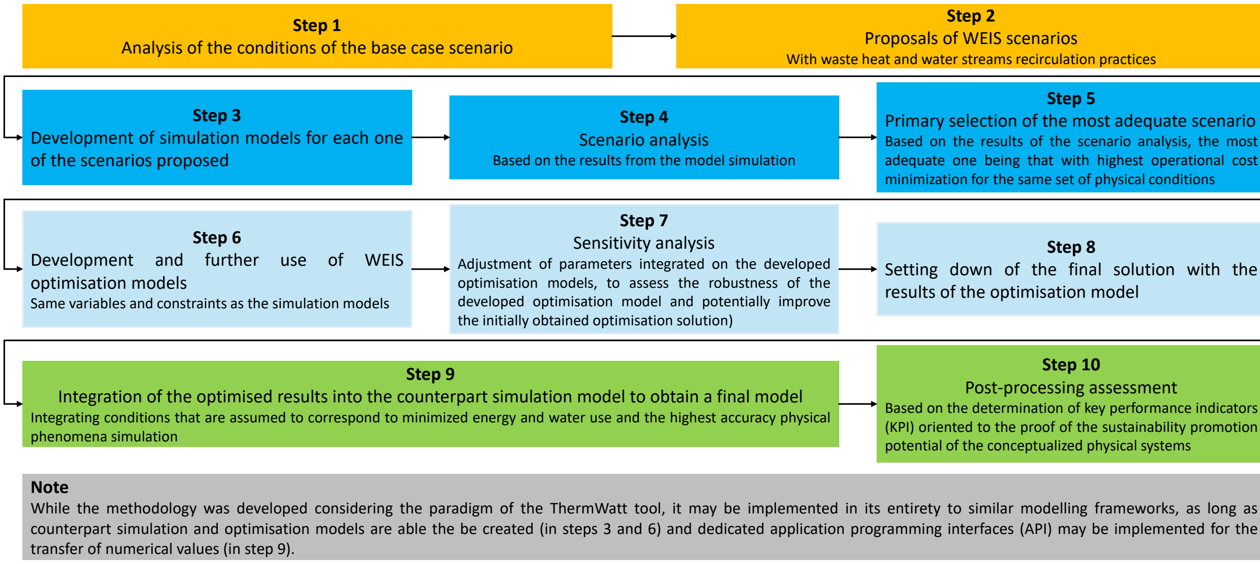

Figure 1. Methodology for model integrity assessment

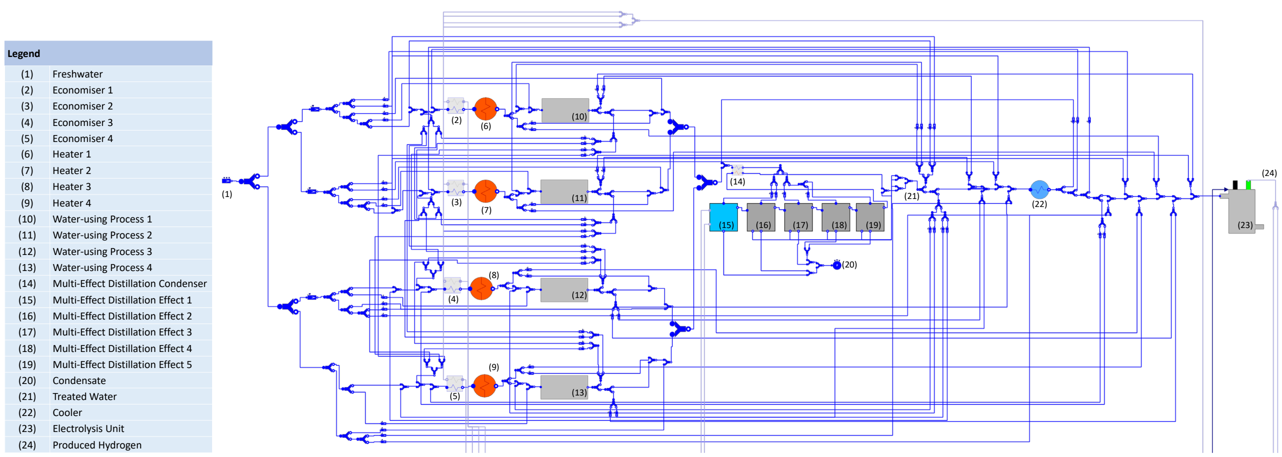

Figure 2. Water system side of both WEIS Scenarios 1 and 2 for Case-study 1 (flowsheet-based model created using the capabilities of the ThermWatt tool)

to proceed with the most accurate analysis of the physical phenomena inherent to these systems and the assessment of the sustainability promotion potential of these.

In this work, the methodology developed for the purpose of assessing the integrity of WEIS models is extensively presented. A set of results related to two case-studies within the Portuguese process industry (namely a ceramic plant) are presented and furtherly used to prove the applicability of the developed methodology.

METHODOLOGY

The assessment of the potential implementation of Water and Energy Integration Systems (WEIS) must subsist on a methodology that is set to allow the whole process from the initial analysis of a case-study (which is commonly a process industry plant and its whole system comprising energy sources, energy supply, energy demand and energy-using processes) to the obtainment of indicators reflecting the sustainability promotion potential brought by the implementation of such systems. In the context of the integration of computational model (which has been the main form of study of the implementation of WEIS, owing to the mostly still conceptual nature of these systems), the implementation of such methodology requires the development of validated and useful models. As such, the delineation of such methodology requires that this is not only one oriented to the assessment of the potential implementation of WEIS Engineering projects but also to the evaluation of the integrity of computational models of these systems.

In Figure 1, the methodology inherent to the process of WEIS model integrity evaluation (and, in this prospect,

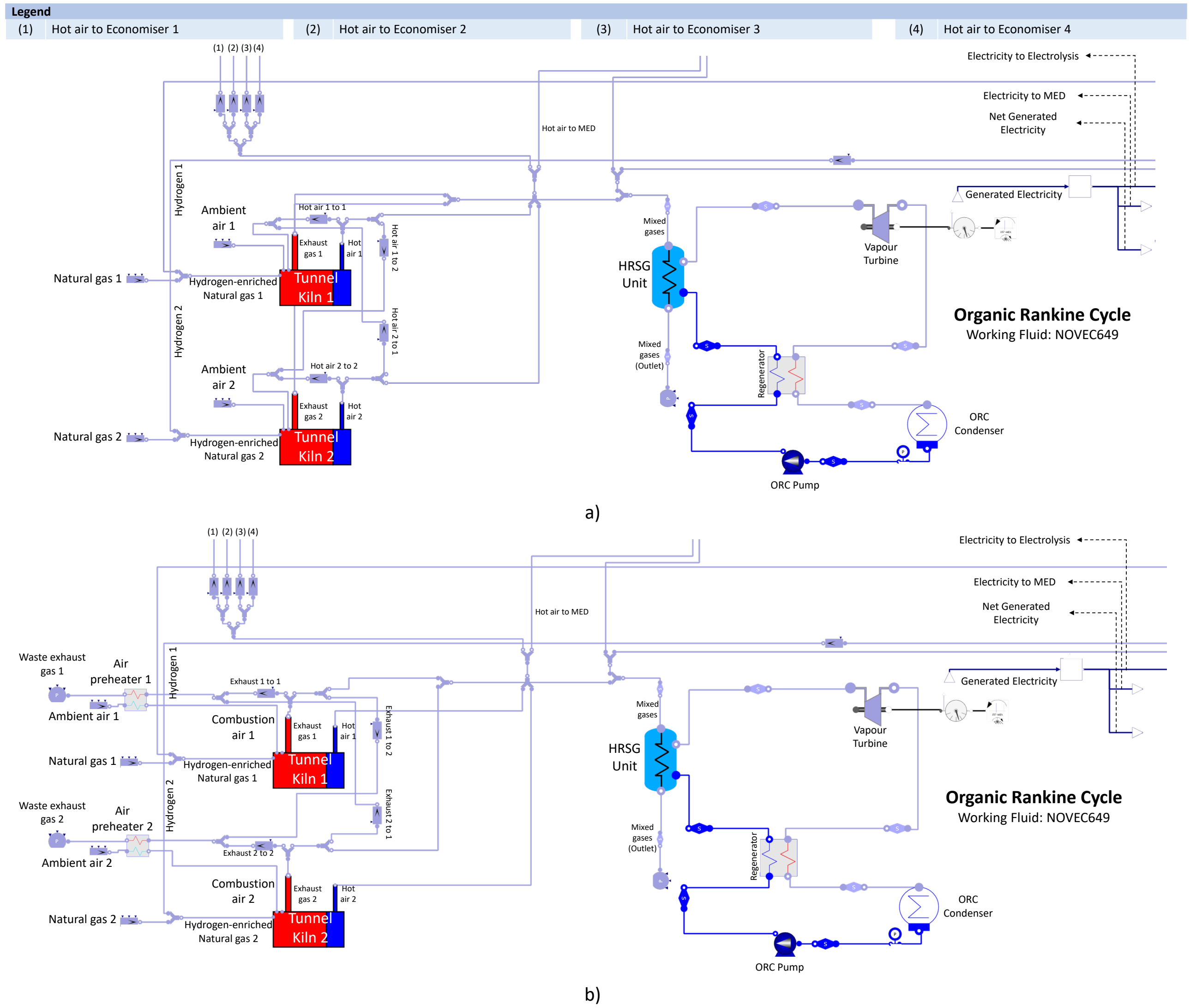

Figure 3: WEIS (Thermal system side) a) Scenario 1 and b) Scenario 2 for Case-study 1 (flowsheet-based model created using the capabilities of the ThermWatt tool)

the assessment of the potential implementation of WEIS within specific case-studies) is extensively detailed.

The development of all the previous works within the overall topic of Water and Energy Integration Systems [2, 3] have subsisted on the application of the afore identified methodology in a subtle manner. The delineation of this methodology which serves as the main subject of this work serves as a manner to turn accessible the implementation of the WEIS paradigm by interested parts of scientific communities, as well as interested parts from end-use sectors representatives.

In the prospect to assess model integrity, the methodology delineated in Figure 1 must be implemented in an aggregated manner, in which the application of each one of the delineated steps converges in the proof of integrity of a developed modelling framework. The quality of a model to be integrate subsists on the verification of the following aspects:

- Simulation-based scenarios must be able to generate most favourable results in comparison to the base case scenarios;
- Optimisation results must be overall more favourable in comparison to the results generated by running of the corresponding simulation models;
- Models are valid, according to the comparison between real-life and simulation data;
- The sustainability promotion capacity (economic, environmental and social pillars) associated to WEIS implementation must not be compromised by the application of the overall modelling framework.

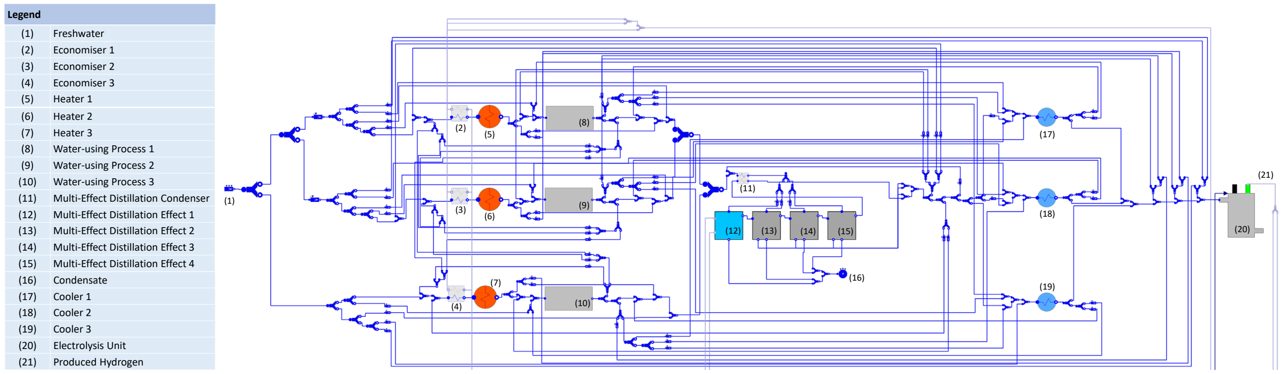

Figure 4. Water system side of both WEIS Scenarios 1 and 2 for Case-study 2 (flowsheet-based model created using the capabilities of the ThermWatt tool)

BACKGROUND

In the prospect to perform a proof of concept of the WEIS paradigm, a set of two process industry-oriented case-studies have been approached. Both these case-studies are set in a Portuguese ceramic plant, has been exploited through the development and further use of simulation and optimisation models (integrated in the ThermWatt computational tool), followed by a complex post-processing assessment based on the evaluation of the viability associated to proposed WEIS.

The afore proposed methodology has been implemented for both case-studies (up until step 3). For both case-studies, the conceptualized WEIS consider the implementation of:

- An Organic Rankine cycle (ORC) to generate electricity;
- A multi-effect distillation (MED) unit for removal of contaminants (salts) from wastewater streams (and thus to produce treated water streams with negligible concentration of contaminants);
- An Electrolysis unit to produce hydrogen streams from treated water streams, which are then blend with the natural gas fuel streams at the inlet of the combustion-based processes.

For case-study 1, the conceptualized WEIS specifically considers:

- A steady-state perspective (owing to the inexistence of combustion-based processes operating in batch);
- Two tunnel kilns as combustion-based processes;
- Four water-using lines (each one encompassing a heater and a water-using process), which are mixed in single water-using line which is then cooled down in a cooler;
- The recirculation of the waste heat streams (either exhaust gas or hot air) to constitute additional energy inputs in combustion-based processes with direct mixture with inlet combustion air (Scenario 1) or by the implementation of air preheaters (Scenario 2).
- For case-study 2, the conceptualized WEIS specifically considers:
- A transient-state/ dynamic perspective (owing to the existence of batch combustion-based processes);
- Four combustion-based processes, two tunnel kilns and two intermittent kilns;
- Three water-using lines (each one encompassing a heater, and a water-using process and a cooler);
- The recirculation of the waste heat streams (either exhaust gas or hot air) to constitute additional energy inputs in combustion-based processes with direct mixture with inlet combustion air;
- The aforementioned streams are also recirculated to a phase change material (PCM)-based thermal energy storage (TES) unit, which is heated up by the passage of the exhaust gases (Scenario 1) or hot air (Scenario 2) streams (while the intermittent kilns are not operating) and from which thermal energy is discharged by the passage of an ambient air stream which is then distributed to each one of the four combustion-based processes.

Each one of the WEIS scenarios developed for case-studies 1 are pictorially presented in the sequence of Figures 2 and 3. Each one of the WEIS scenarios developed for case-studies 1 are pictorially presented in the sequence of Figures 4 and 5.

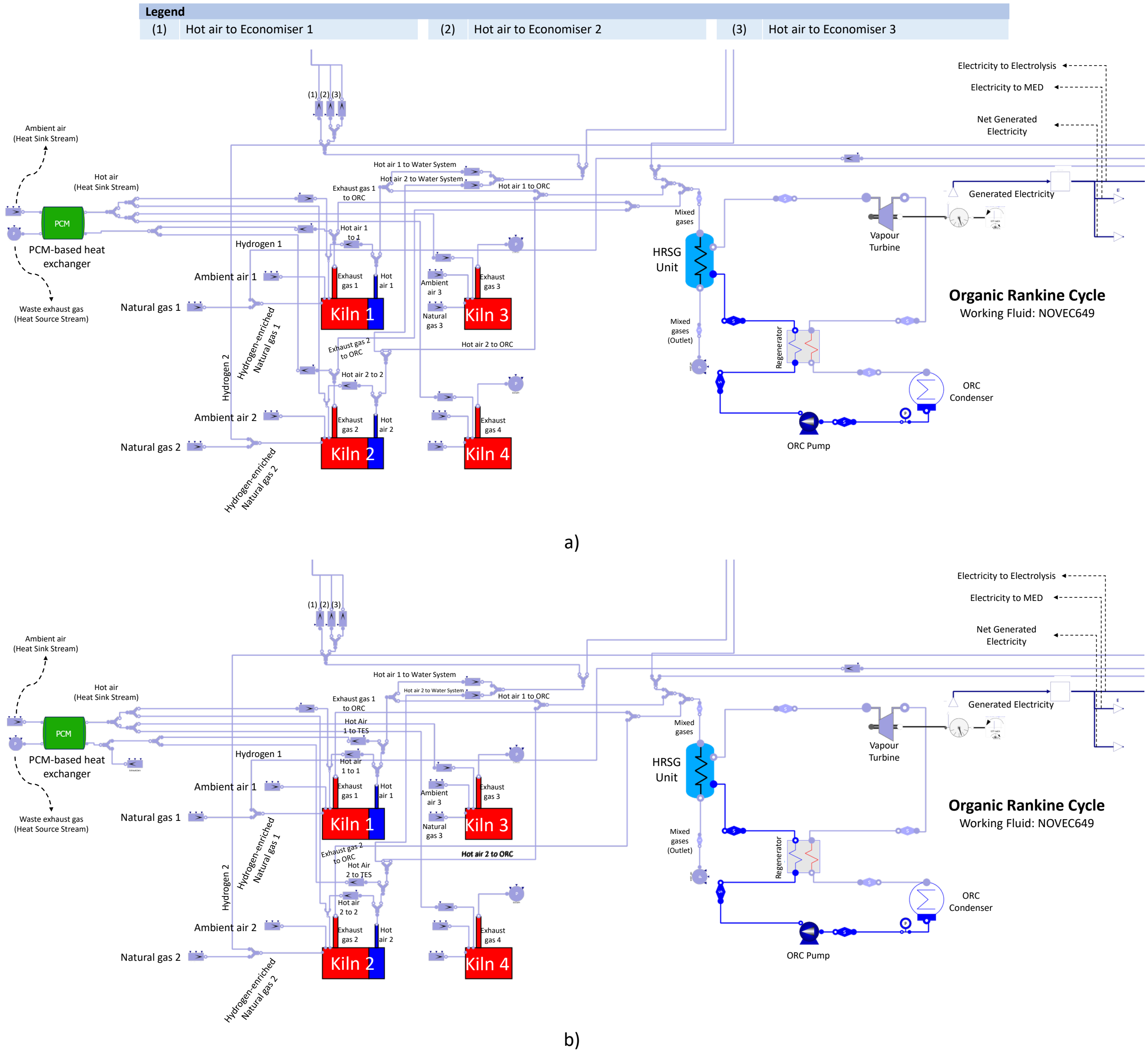

Figure 5. WEIS (Thermal system side) a) Scenario 1 and b) Scenario 2 for Case-study 2 (flowsheet-based model created using the capabilities of the ThermWatt tool)

MODEL INTEGRITY ASSESSMENT

The assessment of model integrity associated to each one of the approached case-studies may be performed by the analysis of aggregated results. In this case, the results which may be analysed in aggregated manner and thus allow the attainment of the specific objectives of the implementation of the afore presented methodology are the energy use or production associated to each one of the energy sources of interest (natural gas use in combustion-based processes, net electricity generation, freshwater consumption and hot/ cold utility consumption), as well as the total operational costs attributed to the overall inputs of energy and water. In the context of the integration of developed computational models, the following sets of results are set to be considered for analysis:

- Base cases;
- Simulation results for each WEIS scenario;
- Initial Optimisation results obtained by the running of the developed optimisation models before sensitivity analysis;
- Optimisation results obtained by the running of the

Table 3: Model integrity assessment for each one of the approached case-studies

Case-study 1	Case-study 2
• Scenario 1 is favoured in relation to scenario 2, owing to the relatively lower operational costs; • It is possible to verify that the obtained values for the hot utility consumption in heaters 1, 2 and 3 are higher in the context of the final model, being slightly higher than the null values obtained by the previous two sets of optimisation results. Such is attributed to the different temperature of the water streams at the inlet of the mentioned three heaters on the final model, which results from the mixture of several recirculated water streams within the whole water system within the overall WEIS; • These temperatures values are slightly lower on the final model (developed in the Modelica language) in relation to the optimisation models (developed with the Python languages), owing to the different modelling packages used to simulate water properties in both categories of models. Such slight decrease of temperature at the inlet of the heaters are responsible for a slight requirement of hot utility supply to achieve the objective temperature values at the outlet of the heaters.	• Scenario 2 is favoured in relation to scenario 1, owing to the relatively lower operational costs (as may be verified by the operational costs associated to the thermal process systems standalone); • The results associated to each one of the parcels associated to energy use (namely the natural gas consumption in each one of the four kilns) are generally lower in the respective optimisation-based scenarios in comparison to the counterpart simulation-based scenarios (which is according to the expected verifications); • The respective energy use levels are relatively higher in the final model (which also causes the total operation costs to be relatively higher). Such relative increase may be attributed to the respective methods implemented for the modelling of the PCM-TES unit in the optimisation model developed for Case-study 2 and in the equipment-level model implemented within the case-study's system-level model. The latter uses a much more accurate method, based on the finite difference method (FDM) for the modelling of heat transfer phenomena; • The afore delineated verification does not considerably affect overall model integrity. The disparity between the results from the counterpart optimisation and final models may be considered a negligible difference, not affecting the balance between modelling accuracy and attainment of the highest sustainability promotion level for the approached case-study.

Overall

- The implementation of all scenarios for both case-studies is set to generate significant results in terms of reduced energy and water-related operational costs in relation the base case scenario;
- All the sets of optimised scenarios generate more favourable results in comparison the ones obtained by simulation models (proving the primary effectiveness of the developed optimisation models);
- The results obtained after the sensitivity analysis correspond to a point in which the thermal-to-electric efficiency considered to assess potential electricity generation on the optimisation models is reduced in order to ensure that this parameter is certainly higher in the context of the running of the final simulation model;
- The aforementioned verification ensures that the definitive solution is the one associated to the minimum possible level of total operational costs, while still considering the most accurate modelling of physical phenomena. In this sense, the net generated electricity (and thus operational costs savings) is relatively lower after the performance of the sensitivity analysis;
- The final results (optimisation results integrated in the simulation model) correspond to significant operational costs savings, evaluated using a model proved to be accurate in terms of the simulation of physical phenomena.

Consumption (MJ/h)	**Cooler 2**	133.00					
	Cooler 3	17.00					
Overall							
Total Operational Cost (M€/year)		2.53	2.04	2.04	2.01	1.87	1.89

developed optimisation models after the performance of sensitivity analysis;

- Final results obtained by the aggregated model.

In Tables 1 and 2, the aggregated results for each one of the WEIS scenarios of interest are presented. In Table 3, the aspects related to the model integrity assessment process for each one of the approached case-studies are presented.

Overall, model integrity associated to the whole modelling framework developed for each one of the case-studies may be considered to have been secured, attending that:

- All sets of simulation results are considered to be more favourable in comparison to base case scenarios (significant reduction of total operational costs);
- All sets of optimisation results are considered to be more favourable in comparison to the

- counterpart simulation scenarios (considerable relative reduction of total operational costs);

- Models are valid;
- The overall modelling framework allows the attainment of final WEIS configurations that have a secured sustainability promotion capacity.

In the framework of the present work, the implementation of methodology presented in Figure 1 may be considered to have been fully fulfilled by section 3 (up until step 3) and the present section 4 (up until step 9). The sustainability assessment process (corresponding to step 10) is considered to also have been completed in the scope of the overall study inherent to this work, although such process have been mostly presented and extensively exploited in the previous related works developed by the authors [4]. In this prospect, the presentation of a significantly higher detail related to this step is considered to be unnecessary in a standalone perspective of the focus of this work. An extensive model validation procedure have been also presented in previous works (the models approached in this work are considered to be a priori valid in terms of the representation of physical phenomena) [5].

An extensive delineation of the sustainability promotion capacity associated to the implementation of the conceptualized WEIS (in respect to the proof of the attainment of benefits associated to the economic, environmental and social pillars of sustainability) is presented in the digital supplementary material (with information adapted from [5]).

CONCLUSIONS

This work extensively presents the methodology developed for the purpose of assessing the integrity of Water and Energy Integration Systems (WEIS) computational models. Although the WEIS paradigm has been introduced and extensively exploited in previous works, the delineation of the approached methodology is fundamental for the scientific communities and end-use sectors representative to replicate similar sustainability promotion results for case-studies other than the ones that have been already exploited. The existence of such a methodology is important due to the primarily conceptual nature of the WEIS paradigm. As such, the assurance of the integrity of models of this type of systems is essential to proceed with the most accurate analysis of the physical phenomena inherent to these systems and the determination of several sustainability promotion indicators (which is the foremost final objective of these of these models).

From the analysis of aggregated results obtained by the use of computational model created for two Portuguese process industry case-studies, it is possible to affirm that:

- The running of initial simulation models for several WEIS scenarios for a same case-study allow the attainment of significant savings at the level of energy use, water use and total operational costs;
- The running of counterpart optimisation models allows the attainment of significantly more favourable results in comparison to the simulation models, with such attainment process being later refined by the consideration of results obtained after the performance of sensitivity analyses to these models;
- The integrity of the final models (through the integration of optimisation results into the counterpart simulation models, considering a compromise between the accuracy of physical phenomena modelling and optimised results) is not compromised by the allocation of numerical outputs from the optimisation models as inputs on the simulation models.

The proposed methodology may be considered adequate for the whole process of the elaboration of the Engineering projects of a WEIS, from the first step of analysing base case data to the final proof of sustainability promotion. Such is supported by the successful implementation of the delineated methodology in two real-life case-studies, having been proved that the integrity of the developed overall modelling frameworks is secured for both cases.

DIGITAL SUPPLEMENTARY MATERIAL

Digital supplementary material is available at https://psecommunity.org/LAPSE:2026.0021.

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AUTHOR IDENTIFIERS

Author ORCIDs:
Castro Oliveira M: 0000-0002-3649-8838
Castro Oliveira R: 0009-0003-3114-7857
Matos HA: 0000-0001-8128-7346

REFERENCES

1. Walsh BP, Murray SN, O'Sullivan DTJ. The water

energy nexus, an ISO50001 water case study and the need for a water value system. Water Resources and Industry 10:15-28 (2015). https://doi.org/10.1016/j.wri.2015.02.001
2. Oliveira MC, Oliveira RC, Castro PM, Matos HA. The paradigm of water and energy integration systems (WEIS): methodology and performance indicators. Systems and Control Transactions 4:1288-1293 (2025). https://doi.org/10.69997/sct.130880
3. Castro Oliveira M., Castro Oliveira R., Matos H.A. Dynamic simulation and optimisation of water and energy consumption in a ceramic plant: Application of the customised ThermWatt computational tool. *Comput. Aided Chem. Eng.* 53: 2377–2382 (2024) https://doi.org/10.1016/B978-0-443-28824-1.50397-5
4. Oliveira MC, Matos HA. Sustainability and strategic assessment of water and energy integration systems: case studies of the process industry in portugal. Energies 17:195 (2023). https://doi.org/10.3390/en17010195
5. Castro Oliveira M. Simulation and Optimisation of Water and Energy Integration Systems (WEIS): An Innovative Approach for Process Industries. *PhD Thesis, IST* (2023) https://scholar.tecnico.ulisboa.pt/records/KwfdB28dqObhPEiL7RtB3VJ6YxviyXFEhWnt