

SOFTWARE INTEGRATION IN THE DEVELOPMENT OF EXPERT DESIGN TOOL FOR ORGANIC RANKINE CYCLE

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ABSTRACT

The industry and scientific community are calling for a feasible, reliable and accessible tool to perform process design and performance assessment for organic Rankine cycle based heat resource analysis such as geothermal or waste heat during the early conceptual stage of design. In this article an online application, Expert Design Tool (EDT), with expertise for equipment selection and performance assessment is proposed. The aim of developing the EDT is to set up an online engineering tool to aid engineers and researchers in carrying out preliminary design exercises and performance evaluation for energy conversion into electricity using organic Rankine cycle (ORC) systems.

Firstly, the status quo of ORC design tool is discussed and EDT architecture, working principle and developing procedure are examined in detail. Secondly, the development of online EDT is associated with different software. The ORC component models are built in Python language and the fluid properties are obtained from CoolProp database. In addition, the Flask software is utilized to build the web framework and HTML/CSS and JavaScript are used for building user-friendly Graphical User Interface (GUI). Consequently, software integration into online environment is explored as a central task. The EDT is feasible for different level users who do not have to possess specific background knowledge or install any specific software. The online deployment and commissioning of EDT will be beneficial to the development of low-grade thermal energy applications based on ORC technology.

1. INTRODUCTION

Conventional steam Rankine cycles have been widely used to exploit the medium to high temperature (503 K - 923 K) heat sources since the 1970s, while a considerable amount of low-grade energy (303 K - 503 K) is still wasted in gas, liquid or solid form due to the lack of cost-effectiveness (Wang, Ling, Peng, Liu, & Tao, 2013). It is difficult to efficiently convert the low-grade thermal energy from these sources into electrical power by the conventional steam cycle power generation technologies. For the sake of conversion of low-grade heat into electricity, various thermodynamic cycles including the organic Rankine cycle, supercritical Rankine cycle, Kalina cycle, Goswami cycle, and trilateral flash cycle have been proposed (Chen, Goswami, & Stefanakos, 2010). Amongst the different technologies in development, organic Rankine cycle (ORC) is characterised by simple structure, high reliability and easy maintenance, compared with Kalina cycle's complex system structure, trilateral flash cycle's difficult two-phase

expansion and supercritical Rankine cycle's high operating pressure (Bao & Zhao, 2013). Therefore, ORCs are playing an important role in low temperature applications such as industrial waste heat recovery, geothermal power or solar thermal energy (Dickes, Dumont, Legros, Quoilin, & Lemort, 2015). Moreover, it is convenient to combine ORCs with other thermodynamic cycles, such as the thermoelectric generator, fuel cell, internal combustion engine, micro turbine, seawater desalination system, Brayton cycle and gas turbine-modular helium reactor in order to make the best of energy (Bao & Zhao, 2013).

Despite these benefits, modeling, simulation and optimization of ORC systems can be challenging and remain a key focus of ongoing research (Ayachi, Ksayer, Zoughaib, & Neveu, 2014; Quoilin et al., 2011; Wei, Lu, Lu, & Gu, 2008). As for many other technologies, the related research is essential for design, sizing or control purposes of ORC applications. The purpose of developing EDT is to set up an online engineering framework to aid engineers and researchers to carry out preliminary design exercises and performance evaluation for energy conversion into electricity using ORC technology. It is a critical deliverable of Above Ground Geothermal and Allied Technologies (AGGAT) programme which is an industry led research and development initiative being championed by the Heavy Engineering Research Association (HERA) of New Zealand. The AGGAT programme is devoted to providing a readily available platform for its membership to facilitate relevant research and development of low enthalpy geothermal and waste heat recovery field.

The EDT is an interactive tool which incorporates the expertise and judgment of experts with domain-dependent knowledge, for example the information associated with equipment selection and performance assessment. It involves several domains including turbines, heat transfer, control systems, materials/fluids selection and process configurations and will integrate all relevant capabilities into one online platform based on pre-defined process algorithms, evaluated literature data and experimental results. In order to accommodate alternative scenarios such as process philosophies, configurations, heat source, fluid, material, equipment size, and scale of operation, the tool needs a well-programmed infrastructure for technical information management and analysis. The EDT can provide engineers or designers with timely access to relevant data and information during the early conceptual stage of design from an enriched database of technical information and give recommendations on technical decision-making.

2. ORC DESIGN TOOL STATUS QUO

The design of ORCs for different applications is normally related to the process configurations, modeling for

components, and simulation and optimization for a specific ORC system. These works, especially model development, are often time-consuming and the industry and scientific community is looking forward to a feasible, reliable and accessible tool to perform aforementioned tasks.

2.1 Commercial modeling software

There is some available commercial modelling software such as Aspen Plus, SimSci PRO/II, VMGSim, AMESim, Chemcad, AxCycle or Cycle-Tempo for simulation of ORCs. These software packages incorporate pre-designed object-oriented libraries, where the equations are already implemented, and the users just need to connect the components properly and set the relevant parameters in the software environment according to their applications.

This generic software is usually powerful multidisciplinary platforms for multi-domain system modeling and analysis instead of focusing on the thermodynamic cycle simulation or specific ORC design. The operation is sophisticated and it is difficult to employ for users who has no related background knowledge. Most importantly, users need to pay a large amount of money to purchase the licenses, which may lead to negative influence on the budget management at an early development stage.

2.2 Offline design tool

Some researchers are devoted to developing general design frameworks for ORC and the attempts to provide necessary tools have been made with reasonable success which provides a good starting point for further research.

Quoilin et al. (2014) presented an ongoing project to develop ThermoCycle, an open Modelica library for the dynamic simulation of small scale thermodynamic cycles and thermal systems. The components package of the library provided a set of models from the basic cell model to higher-level components commonly used in thermal systems. Rettig and Müller (2015) described a prototype of a prediction tool based on above mentioned ThermoCycle library. The main functionality of the tool was to study the performance of an autonomous operated ORC system including automated startup and shutdown procedures. Dickes et al. (2016) created an open-source library, ORCmKit (ORC modelling Kit), for the steady-state simulation and analysis of ORC power systems. ORCmKit included both component-level and cycle-level models and could simulate different ORC configurations. Ziviani et al. (2015; 2016) developed a general ORC simulation tool named ORCSim which actually was a detailed model developed in Python language within ORCmKit. Pezzuolo et al. (2016) discussed a versatile computer tool (ORC-PD) able to perform the fluid selection and the plant design of ORC units with a certain objective function, for example, maximizing the net electric power for different heat sources' type and temperature.

2.3 Online design tool

Timely access to relevant information is significantly important to engineers and designers especially in the early project phase and the internet is considered to be a powerful platform for collaboration information sharing (Varma, Dong, Chidambaram, Agogino, & Wood III, 1996). An online ORC design tool will remain general and accessible to as many users as possible.

Turboden (2015) which is a company in development and production of ORC turbogenerators provides an online power calculator on its website. It is a simple tool for

preliminary evaluation and can indicate the output power and efficiency. The calculator allows selection among pre-determined heat sources and setting process operating conditions and ranges.

Geothermal Development Associates (GDA) (2016) have developed an online process modelling tool which incorporates five models for different types of geothermal power plant and two of them are created for the binary cycle. However they limits the range of values for heat source temperature and in particular flow rate to high numbers (>2000l/m) which suggests the preference of working on large scale plants only. There are four typical working fluid options, i.e. isobutane, isopentane, R134a, and R245fa, to allow some degree of comparative modelling.

3. EDT ARCHITECTURE

The EDT is an ideal framework which is quite distinct from the commercial software packages or other current available tools for ORC process design and analysis as it caters specifically to the needs of general users on an online platform. The EDT is attempting to integrate expertise from researchers and real data derived from experimental rigs to perform the relevant decision-making process and provide with technical recommendations based on the information.

3.1 Software and database

A full open-source stack is crucial in order to enable public access to the online EDT which can run in a user-friendly environment without any additional software requirement. EDT development involves six kinds of software or database, namely Python, Flask, CoolProp, HTML/CSS and JavaScript (JS), as shown in Figure 1.

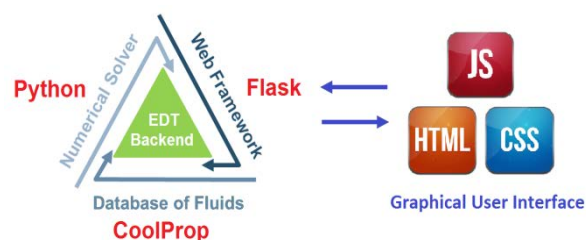


Figure 1: Roles of different software/database during the EDT development.

Basically, three types of software/database are utilized to develop the EDT backend. The central thermodynamic cycle models and ORC component models are built in Python language and the fluid properties are achieved from CoolProp database, while Flask is utilized to build the web framework which is responsible for connecting the EDT backend with the Graphical User Interface (GUI) and GUI development is carried out using HTML/CSS and JavaScript.

Python is characterized by a general-purpose interpreted, interactive, object-oriented, and high-level programming language (Van Rossum, 2007). There are plenty of optional packages for Python applications. Among them, NumPy and SciPy are necessary for the development of online EDT because simulating ORC cycles requires a numerical solver in which the equations of mass and energy balance, heat transfer, pressure drops, mechanical losses, etc. are implemented. In addition, Matplotlib which is a Python 2D plotting library is so critical as to produce high quality figures in complex interactive environments.

The CoolProp library currently provides thermophysical data for 122 pure and pseudo-pure working fluids and its code is written in C++ to utilize modern C++ language features and the functionalities inherent in object-oriented programming (Bell, Wronski, Quoilin, & Lemort, 2014). Moreover, fully featured interfaces have been developed for most programming languages of technical interest, including Microsoft Excel, Labview, MATLAB, Python, C# and EES.

Flask is a lightweight web framework for Python based on Werkzeug and Jinja2 and includes a built-in development server, unit testing support, and is fully Unicode-enabled with RESTful request dispatching and WSGI compliance. Flask enables developers to focus on Web applications or services without having to handle such low-level details as protocols, sockets or process/thread management.

HTML (HyperText Markup Language) is the standard markup language for creating web pages and web applications. With CSS (Cascading Style Sheets) and JavaScript, it forms a triad of cornerstone technologies for the World Wide Web. Web browsers receive HTML documents from a web server or from local storage and render them into multimedia web pages. HTML describes the structure of a web page semantically and originally included cues for the appearance of the document.

3.2 EDT structure

Considering the needs of users and the feasibility, some modules have been planned to be incorporated into the online EDT. A conceptual structure of this design tool is illustrated in Figure 2. Some of these modules have been done and others are still in progress.

Basically there are six modules, namely thermodynamic models, equipment, control, financial, material and web framework. Thermodynamic module is the core of whole application and includes four typical ORC process configurations such as simple ORC, recuperative ORC, thermal oil ORC and two heat sources ORC, while

equipment modules are mainly related to two critical components in ORC systems, i.e. turbines and heat exchangers. Furthermore, the online EDT involves control scheme, financial model and material selection and provides professional analysis and practical advice based on users' concerns. On top of that, web framework need to be well designed and established in order to enable the visit access to general users.

3.3 EDT working principle

EDT is an online application that means any user who has access to the internet can visit it. During the development of EDT, the compatibility with current popular browsers has been taken into consideration and tested in order to ensure the same display effects. The basic working principle is shown in Figure 3.

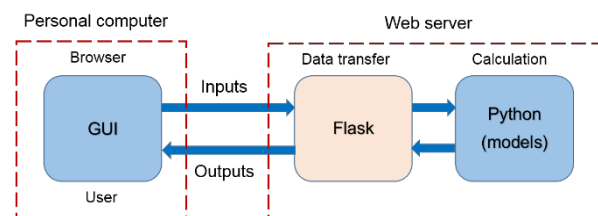


Figure 3: Schematic diagram of the online EDT.

The GUI is the user-end of online EDT. When users visit EDT website via a certain browser, they are asked to choose one process configuration and then the input page with necessary operating parameters appears. Users can either fill particular values or simply use the defaults. After clicking the calculation button, the request is submitted to web server and Flask checks all the inputs which should be within the pre-defined ranges and transfers them to Python codes to execute related calculations. Next, Flask also returns all the results, such as a variety of data and figures, to GUI and the local browser will show a technical report resulting from the received information in the result page.

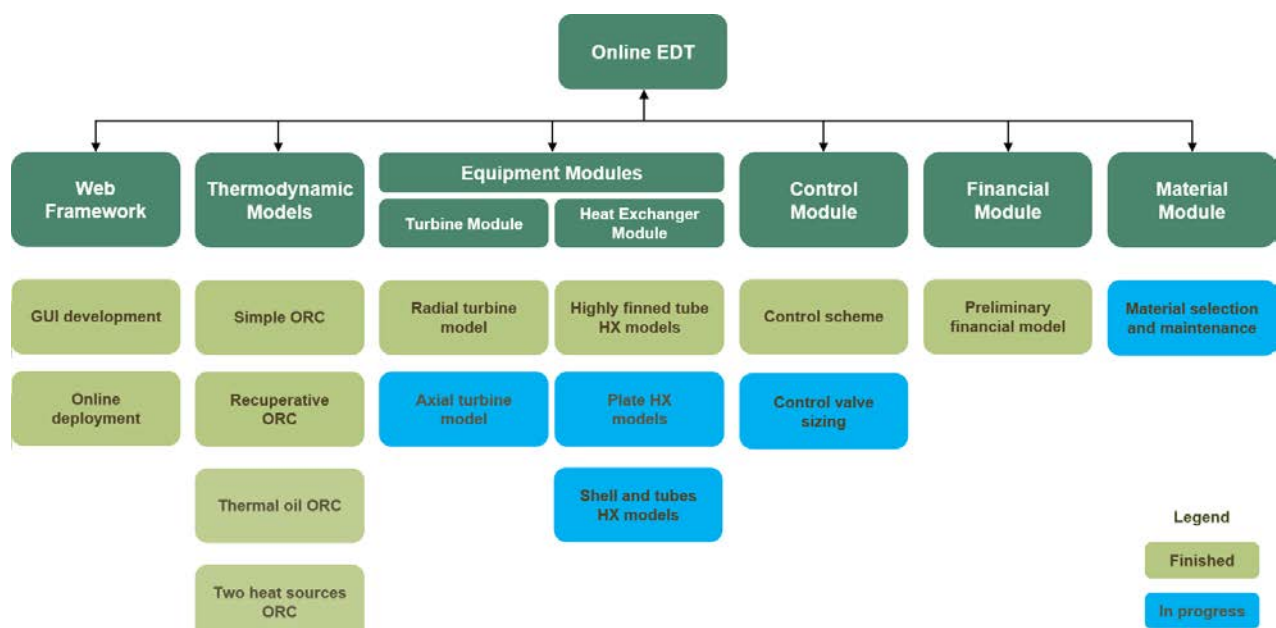


Figure 2: Conceptual structure of the online EDT.

4. SETUP AND APPROACH

The development of EDT is still ongoing and the online EDT will keep updating regularly. Habib et al. (2015) have presented the relevant content about decision-making algorithm, preliminary economic assessment, working fluid screening and model validation. In this article, the main emphasis lays on software integration including modelling, GUI development, and web framework design.

4.1 Modelling

The normal need of most industrial entities is to evaluate the feasibility of ORC for a given heat source (geothermal water, exhaust gas, etc.). Their concerns mainly focus on the potential installed capacity and heat duty as well as a preliminary instruction on the type and size of ORC components. As can be seen in Figure 4, the thermodynamic model for each ORC process configuration plays a dominant role in the online EDT. The results generated by the thermodynamic model will provide the elementary thermodynamic parameters for financial module, control module, material module, equipment selection and geometry design of ORC components.

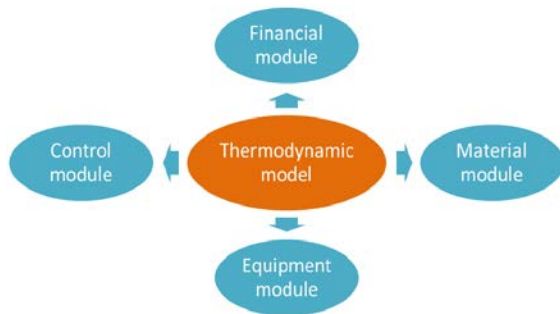


Figure 4: Modelling framework of the online EDT.

The backend of online EDT is consisted of all the models which are implemented in Python 3.4 environment. CoolProp is combined with these models so that the properties of working fluids can be easily retrieved from the database during the calculation process. The thermodynamic models conduct calculations and cycle analysis based on mass and energy balance in terms of users' inputs which specify the operating conditions for a chosen process configuration. Other modules are developed on the basis of the expertise and judgment of experts in AGGAT programme. For example, the highly finned tube heat exchanger is coded based on a series of correlations from Abbas et al. (2015), which are employed to calculate the thermal resistances and pressure drop in the direction of heat flow from the fins side to the tube side. A simplified flowchart for co-current evaporator is illustrated in Figure 5.

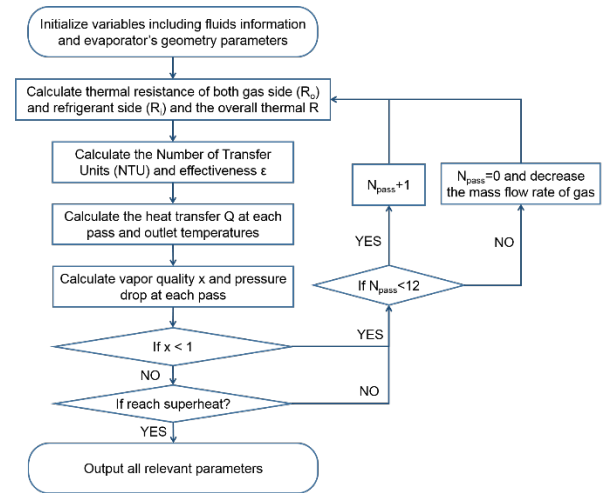


Figure 5: Flowchart of the co-current highly finned tube evaporator.

Currently, the coding for highly finned tube condenser and evaporator in two types, co-current and counter-current have been completed and calibrated against Abbas's Excel calculator. Table 1 shows the results of the counter-current condenser calculated by the Python model while Table 2 indicates the ones generated by the Excel calculator. They are performed under the same conditions, i.e. inlet temperature of cooling medium $T_{c_in} = 20$ °C, inlet temperature of heat source $T_{h_in} = 71$ °C, mass flow rate of cooling medium $m_{cm} = 30$ kg/s and mass flow rate of working fluid $m_{wf} = 2.5$ kg/s. Where Q is overall heat transfer at each pass, h_i is heat transfer coefficient at the inner side, h_o is heat transfer coefficient at the outer side, U is overall heat transfer coefficient, A is contact area, x is outlet vapor quality of working fluid for each pass, x_{avg} is average vapor quality of working fluid for each pass and T_{c_out} is outlet temperature of cooling medium. The difference between these results is quite small, which indicates heat exchanger models can produce reasonable and reliable results and are suitable for the EDT application.

4.2 GUI development

Users interact with the online EDT via GUI which is the only object that users can directly observe and operate. We have devoted to providing a concise and user-friendly interface for different level users. Even if the users have not any background knowledge about ORC, they could also explore this tool by using the defaults. The results of different modules are exhibited in turn in the technical report.

Table 1: Results of the counter-current condenser calculated by the Python model.

Pass No.		$Q(J)$	$h_i(W/(m^2 \cdot K))$	$h_o(W/(m^2 \cdot K))$	$UA(W/K)$	x	x_{avg}	$T_{c_out}(^{\circ}C)$
Pass 1	1st group	4773.48	965.91	53.50	123.49	0.4569	0.7285	34.82
	2nd group	5299.85	926.88	53.26	120.49	0.3816	0.6908	29.76
Pass 2	1st group	1972.12	552.80	52.77	87.23	0.1746	0.3157	24.15
	2nd group	1941.77	476.63	52.65	78.67	0.1035	0.2426	22.06

Table 2: Results of the counter-current condenser generated by the Excel calculator.

Pass No.		$Q(J)$	$h_i(W/(m^2 \cdot K))$	$h_o(W/(m^2 \cdot K))$	$UA(W/K)$	x	x_{avg}	$T_{c_out}(^{\circ}C)$
Pass 1	1st group	4776.63	965.55	53.52	123.51	0.455	0.7273	34.80
	2nd group	5301.10	925.83	53.28	120.46	0.379	0.6893	29.74
Pass 2	1st group	1968.06	550.16	52.78	86.97	0.173	0.3137	24.12
	2nd group	1921.48	470.03	52.42	77.81	0.104	0.2411	22.04

HTML/CSS and JavaScript are the major tools used to develop GUI. HTML can describe the content of web pages while CSS contains versatile pre-defined styles for web pages, including the design, layout and variations in display for different devices and screen sizes. In addition, JavaScript is used to realize some specific interactions, for instance when changing the inlet temperature of heat source or cooling medium, the working fluid list will update automatically but remain the default value “R245fa” if it is still in the list.

After a certain process configuration is chosen by users, an input page with the corresponding process diagram will emerge, as shown in Figure 6. A set of parameters should be specified in order to determine the operating conditions for the chosen cycle and employ the corresponding thermodynamic model to produce relevant results. For the simple ORC process configuration, the input parameters and defaults are listed in Table 3. If a users’ input is out of the set range of a certain parameter, an error message will arise to indicate the rational range.

Simple ORC

Enter data into the text fields. Components can be selected by clicking on a component on the process diagram. When ready, click "Generate technical report" to continue.

Please select the heat source

Exhaust gas ☒

Inlet temperature of the heat source, °C

400.0

Flow rate of the heat source, kg/s

2.0

Pressure of the heat source, Bar

1.0

Please select a working fluid

R245fa ☒

Please select the cooling medium

Air ☒

Inlet temperature of cooling medium, °C

20.0

Pressure of cooling medium, Bar

1.0

High pressure of ORC system, Bar

21.0

Low pressure of ORC system, Bar

3.0

Please specify the assumptions for the simulation

Turbine efficiency (%)

85

Pump efficiency (%)

85

Pinch temperature (°C)

5

Super heat temperature (°C)

3

Generate technical report

NOTE: The calculation is performed based on the thermodynamic model according to users' inputs which are also used in equipment module for preliminary design. Coolprop is utilized to determine fluid properties. This tool may be helpful to gain a basic performance evaluation, but things might be quite different from case to case.

Figure 6: Input page of the online EDT for simple ORC.

Table 3: Input parameters and defaults for the simple ORC process configuration.

Input parameters	Defaults
Type of heat source	Exhaust gas
Inlet temperature of heat source	400 °C
Mass flow rate of heat source	2.0 kg/s
Pressure of heat source	1.0 Bar
Type of cooling medium	Air
Inlet temperature of cooling medium	20 °C
Pressure of cooling medium	1.0 Bar
High pressure of ORC system	21.0 Bar
Low pressure of ORC system	3.0 Bar
Turbine efficiency	85 %
Pump efficiency	85 %
Pinch temperatures	5 K
Superheat temperature	3 K

In order to present the calculation results more efficiently, necessary diagrams are included in the technical report. Figure 7 shows a process flow diagram for the simple ORC configuration which includes the temperature, pressure and mass flow rate of each stream and all the information comes from the thermodynamic model.

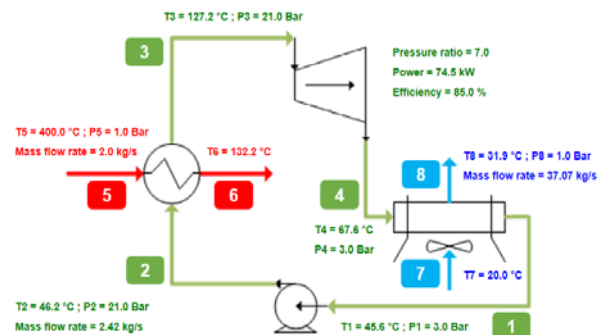


Figure 7: Process flow diagram for a simple ORC.

In addition, it is an essential function to visualize the temperature values and vapor quality for each pass in the evaporator and condenser. The dynamic plotting is achieved by using Matplotlib package in Python environment. Figure 8 and Figure 9 present the schematic diagram, the temperature and vapor quality curve in evaporator design.

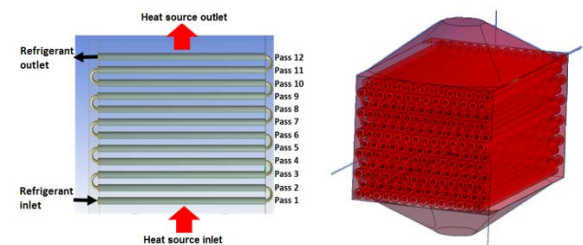


Figure 8: Schematic diagrams for one row and for the whole evaporator.

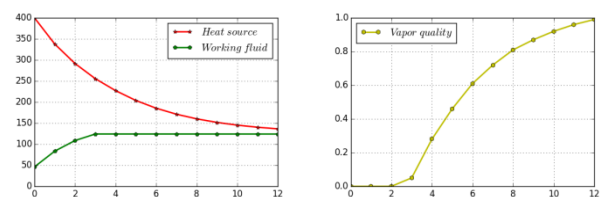


Figure 9: Temperature and vapor quality curves corresponding to each pass of evaporator.

With respect to other modules in the online EDT, Figure 10 shows the preliminary geometry design for radial turbine and Figure 11 exhibits a feasible control scheme for ORC with a thermal oil loop.

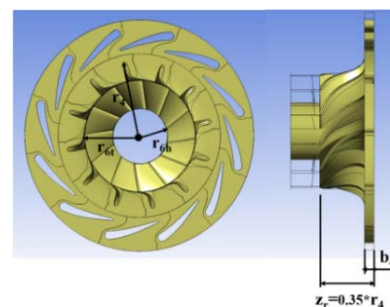


Figure 10: 1D geometry design for radial turbine.

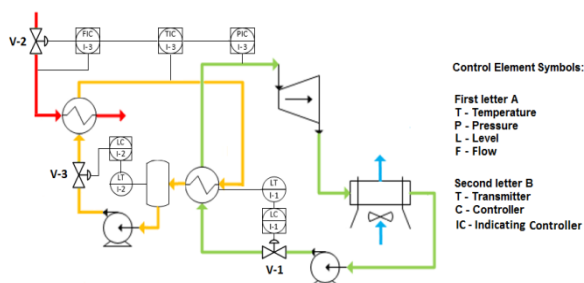


Figure 11: Control scheme for the ORC with a thermal oil loop.

4.3 Web framework design

Flask is an appropriate tool to build the web framework which is just like a bridge connecting GUI and internal models. A key process for this task is to pack all the models into different functions which can be called by Flask and make sure that users' inputs and calculation results can be transferred correctly. In addition, the defaults in input page are set in Flask and the inputs check is done by Flask. Moreover, the plotting function is actually realized in Flask where it is convenient to use the data produced by different models.

Online deployment is a key step for the EDT and many difficulties have been encountered. The EDT is developed on Windows operating system, but web servers usually adopt UNIX or Linux system. In order to establish the Python and Flask running environment on a web server, web server configuration and compatibility issue must be well addressed. Furthermore, port 5000 is the default one during the development stage, while for a formal online application port 80 can be a better choice because port 5000 is often blocked by most firewalls.

5. CONCLUSION AND FUTURE WORK

Currently, most of the modules planned to be included in the EDT have been completed and the EDT has been deployed online. Internal tests are being conducted and modifications will be made according to the feedback. The preliminary version is running well and has demonstrated its capability to provide reliable results and analysis reports. During the development of the online EDT which involves six kinds of software or database, software integration is examined as a key task in order to ensure the feasibility, compatibility and functionality of this tool. The online EDT is intended to be a feasible, reliable and accessible tool to perform preliminary design exercises and performance evaluation for low-grade energy conversion into electricity using ORC technology.

The development of EDT is ongoing. More optional types of ORC components will be developed, validated and combined with the online EDT, such as pump, axial turbine, shell and tube heat exchanger and plate heat exchanger. Optimization algorithms and decision-making process will be explored and refined by means of artificial intelligence methodology so as to provide the most practical and optimal design results in terms of identified performance indexes based on the inference or deduction from plenty of expert knowledge.

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