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Object-Oriented Model and File Format for Heat Exchanger Network Computations

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There have been software packages available for designing, retrofitting and optimising Heat Exchanger Networks (HENs). From those only a handful is available without any charge. Most of them are offered commercially. For professional consultants and large industry such solutions are adequate. However, for researchers they are usually too complicated, not too flexible and expensive. Converting data manually and unifying them in MS-Excel has been practiced to remedy this, but it is time-consuming and leaves a room for errors and semantic mismatch. A step towards a solution of this problem can be an open data exchange file format, which correctly reflects the entities in the HEN domain.
The goal of this contribution has been to develop an object oriented model and a prototype file storage format primarily for HEN related tasks. This file format should enable collaboration on simulation, optimisation and synthesis of HENs. It is based on mapping the relevant process units and stream types to object-oriented concepts. An XML-based file format has been derived from the class design to store the topology and relevant data. To test the object model and the file format, a prototype software application has been created.

1. Introduction

Efficient software tools are essential for research, design and industrial implementation. For process optimisation as well as Process Integration, there have been several attempts to introduce data exchange formats based on XML. Some examples are e.g. electronic document management systems in university context (Costoiu et al., 2012) and the use of ontologies in supply chain optimisation (Silvente et al., 2013).
The benefit of enabling data exchange with preservation of the data structure and model semantics, that the community accepts, can open the door for creating new applications focusing on different parts of the same domain, and at the same time use a common language, for achieving good mutual understanding, saving project cost and increasing scientific and industrial productivity.
A number of software packages for design of Heat Exchanger Networks (HENs) are available. Only several tools are available free of charge and those well-developed are offered commercially. For consultants and large industry such solutions are adequate. For researchers they are usually too complicated, needing a substantial training and too expensive. Data exchange between researchers needed for an efficient collaboration is usually not easy as the software tools are rarely compatible. Using MS-Excel as a data exchange platform, for example, is flexible. However, it is time-consuming and leaves a room for errors and misunderstanding.
Freeware tools have been developed for educational or research purposes. An example comes from the Louisiana State University (Knopf, 2015), available since 2001 – displaying and saving HEN topology. However it has been developed for Windows 95, storing the data in plain text files, without an open specification. Other, more sophisticated, software tools are available. For instance, Heat Integration tool "i-Heat" developed by Process Integration Ltd (i-HEAT, 2015) provides capability to import from or export to process simulators, but inter-operability with other tools of similar purpose or a data exchange format description are limited as the tool is mainly for the in-house use. A commercial tool – SuperTarget®, has been developed originally by Linnhoff March and from the acquisition by KBC (SuperTarget, 2015). It has

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similar features; however being developed as commercial tool for a long time. SuperTarget® software tool can also exchange data with process simulators.
The available commercial and freeware tools for HEN synthesis, optimisation and integration do offer some import-export functionality. However none of them provides an open specification of the data storage formats, which can be established as an essential enabler for the use of those tools and improved efficiency in project teams. The goal of this contribution is to develop an object oriented model and an efficient file storage format for HENs integration and synthesis. This has to adequately describe the information structure and functionalities of heat exchangers, the topology and all relevant HEN properties. They should support the Heat Integration, simulation, synthesis, design of HENs including retrofit. A key goal is to make the model and the related file format open, enabling the exchange of information between research and business partners while preserving of data quality and semantics.

2. Process Integration and Heat Integration Summary

Process Integration serves the industry in solving the challenges posed initially by the oil crises in the second half of 20th century. This is a family of methodologies for combining parts of processes or whole processes together, aiming at reducing consumption of resources or harmful emissions into the environment. It started (Linnhoff and Flower, 1978) mainly as Heat Integration (HI). It has been extensively used in the processing and power generating industry over the last 40 y (Klemeš and Kravanja, 2013).
HI has several definitions, almost always referring to the thermal combination of process streams in continuous or batch processes for achieving heat recovery. The definition of PI, as adopted by the International Energy Agency (Gundersen, 2000) reads as: "Systematic and General Methods for Designing Integrated Production Systems ranging from Individual Processes to Total Sites, with special emphasis on the Efficient Use of Energy and reducing Environmental Effects".

3. The Problem Domain: Heat Exchanger Networks (HENs)

A HI analysis, has a number of steps, including Data Extraction, Pinch Analysis, HEN optimisation, design or retrofit actions, and eventually further iterations until stable results and customer satisfaction are reached. A complete reference on this can be found in (Klemeš, 2013), while Klemeš et al. (2014) provide a textbook university curricula. The parts of the methodology, essential for the current work, include starting from a process flowsheet, performing data extraction, tabulating the process stream data (Table 1). After that the relevant HEN representation – usually as a Grid Diagram, see Figure 1, is constructed.

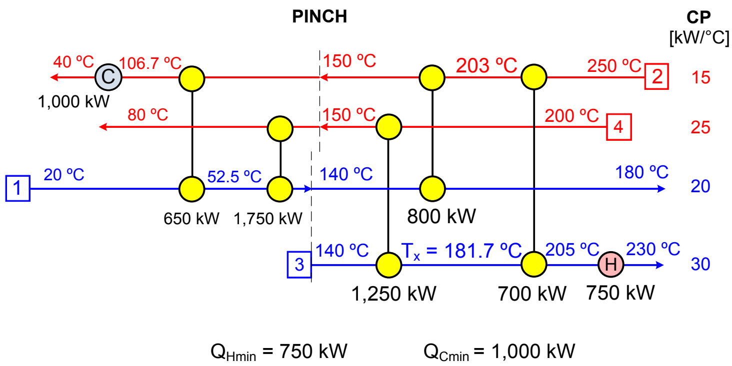


Figure 1: Grid Diagram for the a HEN (adopted from Klemeš et al., 2014)

Table 1: An example dataset for HEN construction

No.	Type	TS [°C]	TT [°C]	CP [kW/°C]
1	Cold	20	180	20
2	Hot	250	40	15
3	Cold	140	230	30
4	Hot	200	80	25

Key concepts in HI are Process Streams and Branches, Utility Streams (hot and cold utilities), Heat Exchanger, Heater, Cooler, Heat Exchanger Network, Temperature Difference, Minimum Allowed Temperature Difference (ΔT_{min}), Splitters and Mixers – to support stream splitting (Klemeš et al., 2013). These and all related concepts have been analysed, proposing consistent conceptual and class models.

4. The Concept and Class Models

First the underlying concepts related to Heat Exchanger Networks are identified, followed by Object-Oriented Analysis and data model identification (Roebuck, 2011), following the steps of finding the objects, organising them, describing their interactions, identifying their behaviour and their sub-items.

4.1 Main Concepts and Relations

The overall concepts mapping is given in Figure 2. Heat Exchanger Network is the container class. It has two members: Id and Name. The name is a free text field which is used to provide an easy to remember key for the system. The description field is optional. Each HEN object has a set of “ProcessingUnit” objects – modelled as a collection based on the Processing Unit class.

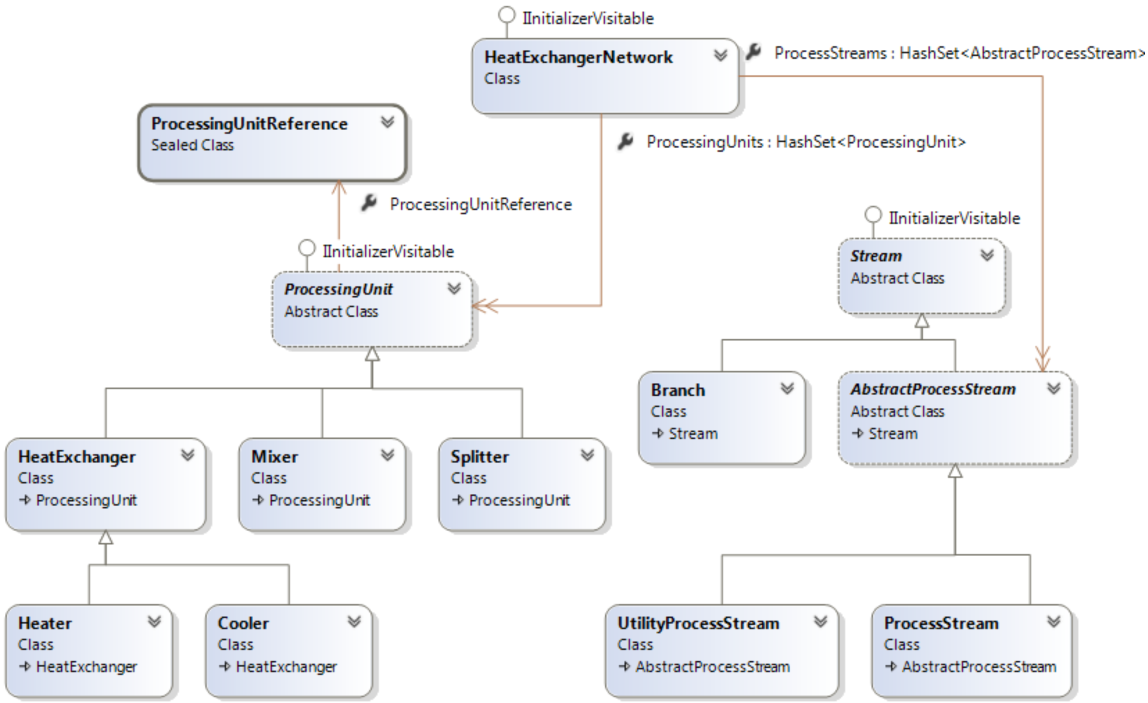


Figure 2: HEN Concepts Model

“ProcessingUnit” is the abstract base class of everything that can modify the state of a stream – including heat exchangers, mixers and splitters. Each “ProcessingUnit” is identified by its “ProcessingUnitReference”. A possible alternative would be to extend this identifier with a “Name” property of type “string” for easier comprehension. Figure 3 highlights the complete “ProcessingUnit” hierarchy.
Process Streams are modelled as a collection of “AbstractProcessStream” objects – normal Process Streams and utilities. The “Branch” class is derived from “Stream” to enable handling stream splits, where “Branch” objects belong to the streams.
Regular Process Streams and utilities have semantic and functional differences. Although nominally each of them has flowrate or heat capacity flowrate (CP) and starting and target temperatures, they are treated differently – all Process Stream properties are usually specified and fixed for the Heat Integration analysis, while the CPs or loads for the utility streams are allowed to vary within certain bounds, providing degrees of freedom in the HEN optimisation. This semantic and functional set of requirements is reflected by firstly defining the “Stream” and “AbstractProcessStream” classes deriving from the latter the “ProcessStream” and “UtilityProcessStream” classes.
The HEN class (“HeatExchangerNetwork”) holds “ProcessingUnit” instances directly and “Stream” only holds references to those “ProcessingUnit” entities using “ProcessingUnitReference” links. They are reflecting the streams passing through the processing unit, which enables specifying the HEN topology. It is sufficient to declare an entity and refer to it avoiding repetition and conflicts. Such data organisation makes the resulting XML, less cluttered and less error prone.
“HeatExchanger” represents recovery heat exchangers, with two “ProcessStream”(s). For utility heat exchangers, “Heater” and “Cooler” classes are derived from “HeatExchanger”, imposing the constraint that

one of the input streams is an “UtilityProcessStream” and the other a “ProcessStream”. They have the same attributes as “HeatExchanger”, but allow implementation flexibility. “Splitter” and “Mixer” classes work in combination with the “Branch” class. A “Splitter” divides a stream into two “Branches”. Two “Branches” can be joined in a “Mixer”. Each “Stream” instance (including “AbstractProcessStream”) can store a list of “Branches”, allowing a “Branch” to have further nested “Branch” instances.

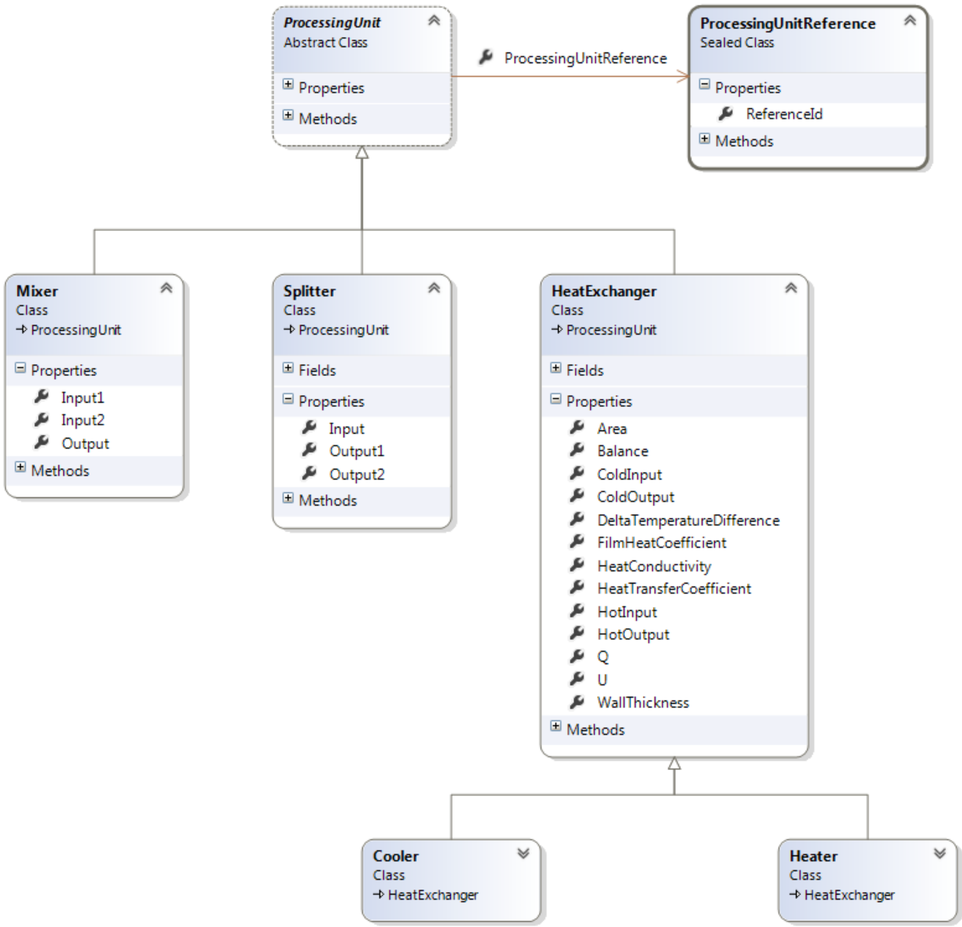


Figure 3: “ProcessingUnits” Hierarchy

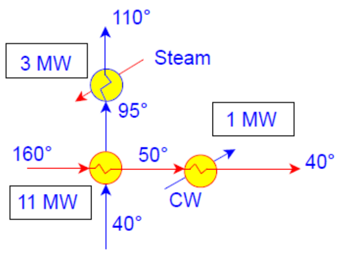


Figure 4: The simple HEN from the Example (after Klemeš et al., 2014)

4.2 Topology Representation

“Stream” is an abstract class containing the attributes of a stream. The key attribute, storing the topology for the stream, is the “ProcessSteps” list. It contains the references (“ProcessingUnitReference”) of the units through which the stream passes. Assume a stream instance “Stream[Id=0]”, having “ProcessingUnitReference[Id=3]”, “ProcessingUnitReference[Id=1]”. This means that the stream enters first Heat Exchanger 3 and then Heat Exchanger 1.

4.3 The resulting XML format

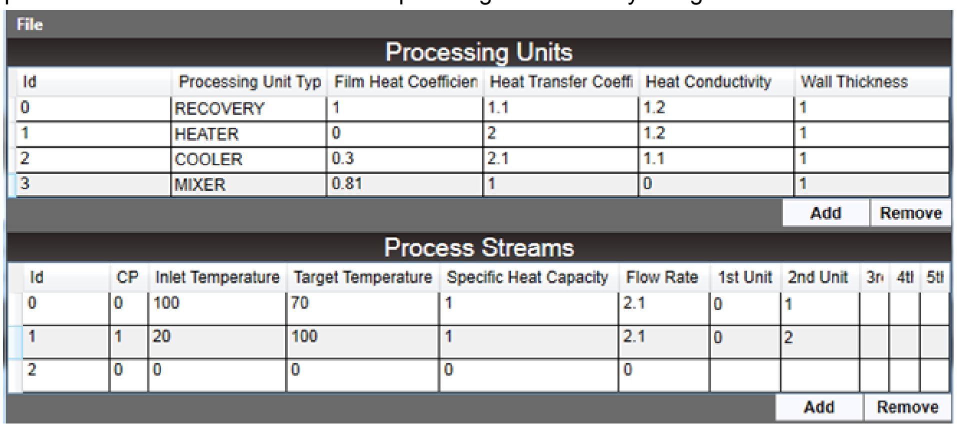
Following the described class system, the “HeatExchangerNetwork” class is instantiated in the root element in the xml document. Taking the simple HEN in Figure 4, Figure 5 shows an XML representation. The first section of the document, after the HEN description, is an inventory represented by the “ProcessingUnits” class. Every unit that is part of the HEN model is a member of the collection. This is followed by the “ProcessStreams” section with embedded stream splits/merges and heat exchanger links.

```xml
<?xml version="1.0" encoding="utf-8"?>
<HeatExchangerNetwork xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xmlns:xsd="http://www.w3.org/2001/XMLSchema" xsi:noNamespaceSchemaLocation="heatExchangerNetwork.xsd">
  <Id>0</Id>
  <Name>TestSystem</Name>
  <Description>Sample network: Two streams, three heat exchangers.</Description>
  <ProcessingUnits>
    <RecoveryHeatExchanger Id="0" FilmHeatCoefficient="2"
     HeatTransferCoefficient="1" HeatConductivity="1" WallThickness="1"/>
    <Cooler Id="1" FilmHeatCoefficient="2" HeatTransferCoefficient="1.2"
     HeatConductivity="1.1" WallThickness="1"/>
    <Heater Id="2" FilmHeatCoefficient="2" HeatTransferCoefficient="1.2"
     HeatConductivity="1.1" WallThickness="1"/>
  </ProcessingUnits>
  <ProcessStreams>
    <ProcessStream Id="0" CP="0.2" SpecificHeatCapacity="2" FlowRate="0.1"
     InletTemperature="40" TargetTemperature="110">
      <ProcessSteps>
        <ProcessingUnitReference ReferenceId="0"/>
        <ProcessingUnitReference ReferenceId="2"/>
      </ProcessSteps>
    </ProcessStream>
    <ProcessStream Id="1" CP="0.1" SpecificHeatCapacity="1" FlowRate="0.1"
     InletTemperature="160" TargetTemperature="40">
      <ProcessSteps>
        <ProcessingUnitReference ReferenceId="0" />
        <ProcessingUnitReference ReferenceId="1" />
      </ProcessSteps>
    </ProcessStream>
    <UtilityProcessStream Id="4" CP="0.199997" SpecificHeatCapacity="4.19"
     FlowRate="0.047732" InletTemperature="20" TargetTemperature="25">
      <ProcessSteps>
        <ProcessingUnitReference ReferenceId="2"/>
      </ProcessSteps>
    </UtilityProcessStream>
    <UtilityProcessStream Id="3" CP="30" SpecificHeatCapacity="2"
     FlowRate="1.48955" InletTemperature="180.1" TargetTemperature="180">
      <ProcessSteps>
        <ProcessingUnitReference ReferenceId="1"/>
      </ProcessSteps>
    </UtilityProcessStream>
  </ProcessStreams>
</HeatExchangerNetwork>
```

Figure 5: The XML representation of the HEN from Figure 4

5. Prototype Software for Validation of the Data Model

A prototype software application has been developed to test the described class model and XML format definition. The application enables users to create and edit HEN descriptions, saving them into an XML file, loading saved work from XML, Grid Diagram view to display topology, and HEN simulation. Figure 6 shows a partial screenshot from a test of the split-merge functionality designed in the XML format.



Id	Processing Unit Typ	Film Heat Coefficien	Heat Transfer Coeffi	Heat Conductivity	Wall Thickness
0	RECOVERY	1	1.1	1.2	1
1	HEATER	0	2	1.2	1
2	COOLER	0.3	2.1	1.1	1
3	MIXER	0.81	1	0	1

Id	CP	Inlet Temperature	Target Temperature	Specific Heat Capacity	Flow Rate	1st Unit	2nd Unit	3r	4tl	5tl
0	0	100	70	1	2.1	0	1			
1	1	20	100	1	2.1	0	2			
2	0	0	0	0	0					

Figure 6: Screenshot of the HEN Editor interface

6. Conclusions and suggestions for future work

This contribution has presented a class model and a suggestion for an XML format for storing HEN related data and enabling efficient data exchange. This is a prototyping effort responding to the challenge of providing distributed research teams with means of exchanging model information with the model semantics accompanying the data in appropriate context. The presented model and XML format are the first step towards fully addressing this challenge. The correctness of the model has been validated using a simple prototype software tool where all key functionalities regarding the data have been verified – including editing, saving, loading and simulating a HEN. It is important to stress that the format allows handling stream splits.

The future work should include evolution of the class model and XML format to more fully integrate stream splits, allowing direct implementation of more than two branches as well as measurement units. Further, the possibility to combine the developed ideas with the CAPE-OPEN initiative (Co-LaN, 2015) should be investigated, potentially providing interfaces and compliance with the CAPE-OPEN compliant software tools on the market.

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