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Enhancement and Energy Optimised Integration of Heat Exchangers in Petrochemical Industry for Waste Heat Utilisation

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Czech-Chinese Project Transmission Enhancement and Energy Optimised Integration of Heat Exchangers in Petrochemical Industry Waste Heat Utilisation is a joint project of Czech Republic, SPIL, Brno University of Technology – VUT Brno and the People's Republic of China, Xi'an Jiaotong University, Xi'an, Shaanxi. The 3 y project contributes to solving the energy situation and reduction of emissions. The use of low-grade heat is an effective means of saving energy and reducing greenhouse gases, which is increasingly sought after both for large companies also in local industrial facilities and even households. It has been increasing the emphasis on the use of low-potential energy results in increased demand for sophisticated heat exchangers. Methods, standards and the creation of modular structures optimised for different outputs based on the practical use of research results are being developed for various sources of waste heat, types of circulating media and technical operating parameters. Layout and construction designs allow designers to professionally design and manufacture suitable heat exchangers for specific conditions of the production process from the very beginning and a wide scope of conditions and requirements. Utility models and software modules were created and supported with research publications.

1. Introduction

Waste heat utilisation has always been a vital issue in various industries (Su et al., 2021), which contributes to the primary energy consumption reduction (Anastasovski et al., 2020). Many advanced approaches were developed for Heat Integration from the view of Total Site (Möhren et al., 2021), innovations for improvement and new development of heat exchangers were proposed (Arsenyeva et al., 2021), and various methods for heat exchanger networks (HEN) optimisation (Zirngast et al., 2021) and HEN synthesis with detailed equipment design (Cotrim et al., 2021) were presented. The project LTACH19033, "Transmission Enhancement and Energy Optimised Integration of Heat Exchangers in Petrochemical Industry Waste Heat Utilisation", aims to further explore the new ideas and technologies for heat transfer enhancement and energy integration to achieve the goal of greenhouse gas reduction. The project is funded under the bilateral collaboration of the Czech Republic and the People's Republic of China. The project partners are Xi'an Jiaotong University, Sinopec Research Institute Shanghai, SPIL VUT Brno, and EVECO Brno sro. The project is also supported by the National Key Research & Development Program of China (2018YFE0108900).

2. Achievements and Deliverables

During the project, three utility models (patents) and four software modules have been planned and delivered in the Czech Republic. Two invention patents and three software modules have been submitted and approved in China. The dissemination has been delivered by publications in journals. They are summarised in this section, referring to the documents of the deliverables.

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1033

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A review paper with the title "Heat transfer enhancement, intensification and optimisation in heat exchanger network retrofit and operation" by Klemeš et al. (2020) was developed for this project. This paper reviews the history and the recent developments in the areas of Heat Transfer Enhancement and the retrofit of HENs, providing a critical analysis from the viewpoint of obtaining practical solutions with positive cash flows while minimising the issues related to operability – emissions, flexible operation and control. The analysis clearly shows the need to focus future research and development efforts on increasing model fidelity and practicality, addressing operability issues, and, most importantly – developing flexible and efficient tools for communicating optimisation results to industrial practitioners and plant managers who would implement the process retrofit recommendations.

2.1 Method for designing, operating and retrofitting Heat Recovery Networks

HEN synthesis and retrofit are the main issues that this project is focused on. One concentration was developing methods for HEN topology modification. Many novel methods which are based on the Pinch Analysis, and more specific based on the Grid Diagram were proposed. A two-stage method has been developed based on the structure of Shifted Retrofit Thermodynamic Grid Diagram (SRTGD) (Wang et al., 2020). First, the data of an existing HEN should be gathered to draw an STRGD. Then these data were input in a mixed-integer linear programming (MILP) model developed based on the structure of STRGD. The model with the objective function of minimising total utility cost and the approximate capital cost was solved by the Gurobi solver to get the optimal solution. At this stage, resequencing, re-piping and adding heat exchangers were considered. Next, the particle swarm optimisation (PSO) optimised the inlet and outlet temperatures of each heat exchanger based on the structure obtained by the MILP model. The temperatures of heat exchangers in the solution of the MILP model were inputted in PSO as the particle in the initialisation. The positions of particles evolved during the iteration of the PSO. Finally, when the convergence criterion was satisfied, the HEN retrofit plan was obtained. The results showed that the proposed method can significantly reduce the total annual cost of the cases.

Wang et al. (2020b) extended the SRTGD by proposing an SRTGD with the Shifted Temperature Range of Heat Exchangers (SRTGD-STR). This contribution enables the heat exchanger type selection when retrofitting HEN. The temperature ranges of several widely used heat exchangers are integrated into the SRTGD for easy type selection. Besides the temperature range of heat exchangers, the material types also have an influence on the investment of new equipment and leading to different design plans. Wang et al. (2021b) further extended the SRTGD by proposing an SRTGD with Shifted Material Temperature Range (SRTGD-SMTR) tool which can analyse and diagnose the existing HEN to determine feasible retrofit plans with pre-selected heat exchangers and materials. Then the constrained PSO algorithm was developed to minimise the total annual cost.

Wang et al. (2021c) proposed a method to consider prohibited and restricted matches in the synthesis of HENs. The method is based on the Advanced Grid Diagram, and the trade-off between the cost brought by the potential risk and the benefit of the heat exchange was compared and illustrated by the Benefit Diagram.

Chin et al. (2020) extended the HEN retrofit to a long-term issue. The lifetime of heat exchangers and reliability functions were considered in the HEN structure retrofit. A Mixed Integer Linear Programming (MILP) model based on the work of Wang et al. (2020) was proposed for HEN retrofit and maintenance planning. The decisions such as heat exchanger upgrade, purchase, replacement, maintenance can be made.

Another way for HEN retrofit is heat transfer enhancement (HTE), and some achievements have been done in this project. Li et al. (2021) developed a target-evaluation method with the consideration of the thermal efficiency and the level of heat transfer enhancement for energy-saving. The energy target is implemented by the SRTGD to determine the grassroots thermal design parameter. A simple performance plot for the HTE evaluation with a simple calculation was performed. Although energy consumption reduction and total cost minimisation are always the main targets in the HEN synthesis and retrofit, another important issue in Heat Integration is the risk, which is reflected in the prohibited or restricted matches in the design of HENs.

In the operation of HEN, heat exchanger leakage can sometimes happen, which will disrupt production, increase the total annual cost, and threaten the safe operation of equipment. To quantitatively taken the leakage risk characteristic in the HEN optimisation, a mathematical programming model was proposed by Wang et al. (2021d). This model considers the risk severity and mean occurrence frequency, and takes the risk cost with the operating cost and investment cost in the objective function. The results can illustrate the turning points which might change the HEN topology when the risk level increased.

In hybrid energy systems, heat and power can be minimised by using some tools. Wang et al. (2021a) developed a Heat and Power Composite Curve (HPCC) based on the Pinch Analysis concept to visualise the heat, power, and total energy requirements in a hybrid energy system. This Composite Curve can show the electricity that is stored should be purchased and generated by the system.

1034

2.2 Heat exchanger equipment development and investigation

The technical solution relates to a spiral heat exchanger intended for use in the petrochemical, power, and other industries (SPIL team, 2019) has been developed. The proposed heat exchanger design maximises the heat transfer efficiency while minimising the pressure drop. According to the invention (utility model), each partition consists of an inner part and an outer part placed around it; the outer part is located between the inner surface of the jacket wall and the outer circumference of the inner coil and inner spiral parts. A perforated partition is formed between the central support tube and the inner periphery of the outer spiral portions. The baffle assembly is formed to form a continuous spiral surface along the entire length of the internal space of the exchanger with the central support tube. The perforated baffle system increases turbulence and hence the heat transfer coefficient, but with less than normal pressure drop, as the continuous surface of the baffle improves the flow of the heat transfer medium through the interior heat exchange space. Improved flow also has a positive effect on reduced contamination during operation, and thus reduced downtime, cleaning or even replacement of the internal piping system.

The innovation actions have resulted in a Utility Model entitled "**Tubular heat exchanger with spiral baffles** and increased efficiency". The subject of the utility model is a vertical tube heat exchanger with spiral baffles to increase the efficiency of heat transfer, corrosion resistance and clogging and extend its life. This type of vertical tube heat exchanger maintains the increased efficiency of a conventional horizontal tube heat exchanger even in cases where, due to the required direction of media flow and/or spatial disposition, the horizontal tube heat exchanger cannot be used. The openings in the baffles prevent uneven settling of dirt and improve the efficiency of heat exchange between the outside of the tube bundle and the inner surface of the casing. The spacer strip mechanically strengthens the partition but also effectively reduces the space between the outer side of the heat exchange tube bundle and the surface of the inner wall of the exchanger shell. The application areas of the utility model include industries such as petrochemistry, energy, metallurgy, cooling, seawater desalination, and has a high potential, while the growing need for the use of low-potential thermal energy increases the possibilities of using this system even in cases where it was not economically advantageous. The advantages of the developed design include:

- There is a significant increase in the heat transfer coefficient, in particular by increasing the turbulent flow, which increases the heat transfer coefficient on the pipe surface.
- The continuous baffle has no non-functional areas and therefore improves the flow in all directions.
- The pressure loss inside the casing is effectively reduced and, thanks to the possibility of multi-surface design, the passage of the medium through the exchanger is streamlined.

A utility model of specialised equipment was created, "**Compact units for ammonia production**". The device, according to the utility model, is designed for the production of ammonia in plants with a flue gas cleaning system that uses ammonia as a reagent for DeNO_x systems. The main benefit of the technology is the reduction of the costs of these operations for the elimination of ammonia as a dangerous substance. The device uses the conversion of a solution of technical urea to ammonia under specific conditions (temperature and pressure). When the urea solution boils at that temperature, a hydrolysis process takes place, and urea forms ammonia gas, water vapour and by-products. The overall chemical reaction takes place according to the following equation: $CH_4N_2O + H_2O \rightarrow 2NH_3 + CO_2$. The produced ammonia can then be used in downstream process units for supplying the SCR (Selective Catalytic Reduction) or SNCR (Selective Non-Catalytic Reduction) systems to reduce nitrogen oxides in the flue gas. The advantage of using ammonia in this way, compared to technical urea solution, is the higher efficiency of DeNO_x systems, which is very important considering the tightening emission limits of combustion plants. In the utility model, it is advantageous to heat the vessel with waste heat from the flue gas, possibly a by-product from an associated operation (steam, thermal oil).

Guo et al. (2021) developed a numerical method was established to investigate the characteristics of ash deposition in tube bundle heat exchangers. An integrated fouling model including transport, rebound, deposition, and removal of particles was employed to predict the behaviour of particles. Then, the effects of particle diameter and flue gas velocity on collision mass, deposition mass, absolute deposition ratio, and relative deposition ratio were studied. At last, the thermal-hydraulic and ash deposition characteristics of three different tube shapes were compared.

Cao et al. (2021) applied the theoretical analysis and numerical simulation method to compare the aerodynamic noise and heat transfer in shell-and-tube heat exchangers with continuous helical and segmental baffles. The results show that with the increase of Reynolds number, several parameters such as the sound pressure, the pressure drop per unit tube length, and the Nusselt number all increase. The average synergy angle of continuous helical baffles is 11 % lower than that of segmental baffles, which corresponds with 23 - 37 % lower sound pressure.

Chen et al. (2020) developed a water-water heat transfer experiment system to study the baffle patterns such as tri-flower baffle, pore plate baffle, rod baffle, segmental & pore baffle, and segmental baffle on the heat

transfer and fluid flow characteristics of shell-and-tube heat exchangers. Results showed that rod baffle, triflower baffle, and pore plate baffle have better performance than segment baffles.

Li et al. (2020) compared the diverse baffled longitudinal flow shell-and-tube heat exchangers (STHX) and segmental baffle shell-and-tube heat exchanger (SG-STHX) from the perspectives of entropy generation, exergy destruction, and efficiency evaluation criterion. Results showed that longitudinal flow pattern has better performance on energy saving, especially for the rod baffle shell-and-tube heat exchanger (RB-STHX).

2.3 Heat storage solutions

Chinese invention patent: Hydrated-salt-based medium-and-low-temperature chemical heat storage material and preparation method

The invention discloses a preparation method of a hydrated-salt-based medium-and-low-temperature chemical heat storage material. The obtained hydrated-salt-based medium-and-low-temperature chemical heat storage material has better thermochemical properties than hydrated-salt-based medium-and-low-temperature chemical heat storage materials in the prior art. Three hydrated salts with different characteristics are mixed to a specific weight ratio, the preparation method provided by the invention is utilised, the finally synthesised ternary hydrated-salt-based heat storage materials in the prior art in thermochemical properties such as adsorption power performance, heat storage density and cycling stability, and can effectively avoid a series of problems which are easy to occur in gas-solid heat storage reaction processes such as agglomeration, expansion, deliquescence, leakage and the like. The feasibility of the hydrated-salt-based composite thermochemical heat storage material in a medium-and-low-temperature chemical heat storage system is greatly improved. The patent has been approved by China National Intellectual Property Administration with the grant code ZL 202010759968.8.

On the Chinese side, a patent titled System and method for combining power generation, heat supply, refrigeration and water taking based on chemical heat storage has been delivered. The invention discloses a system and method for combining power generation, heat supply, refrigeration and water taking based on chemical heat storage. In the system, a first hydrated salt-based heat storage material absorbs heat to be subjected to a desorption reaction to generate water vapor, or the first hydrated salt-based heat storage material and water from a first valve are subjected to a hydration reaction to release reaction heat, a first power generation unit comprises a first steam turbine doing work through superheated steam expansion and a first power generator coaxially connected with the first steam turbine, a second hydrated salt-based heat storage material absorbs heat to be subjected to a desorption reaction to generate water vapor, or the second hydrated salt-based heat storage material and water from a second valve are subjected to a hydration reaction to release reaction heat, the desorption temperature of the second hydrated salt-based heat storage material is lower than the desorption temperature of the first hydrated salt-based heat storage material, a second power generation unit comprises a second steam turbine doing work through expansion of high-pressure superheated steam and a second power generator coaxially connected with the second steam turbine, and a refrigeration unit is connected with a second circulation loop through a three-way valve for refrigeration. The patent has been approved by China National Intellectual Property Administration with the grant code ZL 202010972093.X.

Li et al. (2021a) used expanded graphite (EG) as supporting matrix to impregnate LiOH to further improve its heat and mass transfer. Li et al. (2021b) developed a method to improve the thermo-chemical conversion behaviours, including reactive transport processes and output performances of an open thermochemical energy storage (TCES) unit. The local thermal non-equilibrium (LTNE) model was adopted, and the effect of non-uniform porosity was considered. Results showed that the cascaded TCES unit has great potential for performance improvement of the low-grade energy storage system. To keep the balance of supply and demand in domestic heating with renewables, Li et al. (2021c) synthesised the composite sorbents consisting of expanded graphite (EG) and varying mass ratios of LiOH and LiCl with good stability. The study result showed that when salt contents of samples are over 60 wt%, the vapour sorption property can be enhanced, and energy storage density is improved.

2.4 HEX design and optimisation software

A bunch of tools for various types of heat exchanger design and rating, and HEN analysis, design, and retrofit are developed during this project.

The shell-and-tube heat exchanger design & rating software has been designed by the SPIL team for performing heat exchanger calculations and obtaining enhanced heat exchanger designs. The Requirements Analysis phase has identified the necessary data inputs, data outputs and visualisation needs. This was followed by the complete identification of the Use Cases and the algorithms to be followed. The results of the Use Case analysis were then used to design the user interface and the software algorithms. The coding phase implemented the selected software design in VB.NET. The testing has been performed in-house and with the

1036

partners from the Xi'an Jiaotong University. The user feedback has been incorporated into the software code, taking two iterative steps. The development process was completed by writing and publishing the User Guide. **The shell-and-tube heat exchanger design software** developed by the XJTU team has two different design modules. The first is the lubricating oil cooler design module, which is suitable for the design of high-temperature lubricating oil cooler design module, chemical, refrigeration and machinery. The second is the condensing sub-cooler design module, which uses water-vapour and water-water heat transfer to condense the steam discharged from the secondary side of the steam generator into saturated water. The software has been approved by the National Copyright Administration of China with the grant code 2020SR1228282.

The simultaneous optimisation design software for heat exchange networks and heat exchangers developed by the XJTU team supports the simultaneous design of shell-and-tube heat exchangers and HENs. The Bell-Delaware method was adopted for the design of heat exchangers, and the Genetic Algorithm is adopted for simultaneous optimisation. Parameters of heat exchanger structures and networks are set as gene codes, and all the parameters meet the standards of GB/T 151-2014 and Tubular Exchanger Manufacturers Association (TEMA). The software has been approved by the National Copyright Administration of China with the grant code 2020SR1216529.

The Spiral Baffles Shell and Tube Heat Exchanger Design Software Module developed by the SPIL team, or SPIL-HXSB, is a software application that allows engineers to design Shell and Tube Heat Exchangers with Spiral Baffles. It determines a custom solution to meet the specific specification. Engineers can design an exchanger to meet the TEMA standards and user requirements considering flexible shell elements and other specific requirements.

The Waste Gas Compact Thermal Oxidiser Software Module developed by the SPIL team, or SPIL-WGCTO, is another application that allows engineers to design the waste gas thermal oxidiser unit (courtesy of EVECO). Engineers can apply this module to design an oxidiser unit that utilises the heat from the waste gas while ensuring the disposed waste gas is relatively less harmful. The unit consists of a combustion chamber that governs the combustion of waste gas and supply chambers that have provided heat exchange between waste gas and combusted flue gas. The supply chambers have similar characteristics to the concept of shell and tube heat exchangers. This software module determines a custom solution to meet flexible user requirements

The shell-and-tube condenser design software developed by the XJTU team specialises in condenser design. Two modes are available in the software: design and rating. The design mode calculates the heat exchanger tube length and submergence coefficient based on the working condition input parameters, and the rating mode reviews the working condition input parameters based on the existing condenser heat exchanger tube length. The fluid states are pure gas, pure fluid, two-phase state, and automatic identification. The only liquid mode is supported on the tube side, and only the vapour mode is supported on the shell side. The software has been approved by the National Copyright Administration of China with the grant code 2021SR0718580.

The Heat Exchanger Network Retrofit Module developed by the SPIL team, or SPIL-HENR, is the application for engineers to identify the optimal retrofit options in an existing HEN. The existing module requires just the users' input of the cold and hot streams and parameters of the heat exchangers. The module then performs optimisation on the streams and determines the optimal retrofit options for the HEN using a meta-heuristic. The minimum temperature difference constrained is incorporated into the software module. The retrofit structure is optimised with the minimum payback period set as the objective function. This software module determines a custom solution to meet flexible user requirements.

3. Conclusions and future goals

The project LTACH19033 has delivered 16 journal papers, 7 software modules, and 5 utility modules so far. Contributions for energy and emissions reduction are continually proposed.

In the second half-year of 2021, the following tasks are still in progress based on the phases of LTACH19033: publications of more case studies and a confidential joint report for the funding agencies.

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