Dynamic simulations of medium-sized hydrogen liquefiers based on EcosimPro simulation software

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Abstract. Dynamic simulations of medium-sized hydrogen liquefiers have been performed using process simulation software EcosimPro. Two hydrogen liquefier process flows have been simulated. One process flow is a helium refrigerator with one helium turbine providing cooling power for hydrogen liquefier, the other one is a helium refrigerator with two helium turbines providing cooling power for hydrogen liquefier. Control logics and control strategies for these two hydrogen liquefiers have been proposed. The cooling down simulations have been performed separately. One turbine hydrogen liquefier, pressure ratio is 2/16 bara, helium mass flow rate is 111 g/s, hydrogen mass flow rate is 4.3 g/s, the liquefaction rate of hydrogen is about 191 L/h. Two turbines hydrogen liquefier, pressure ratio is 1/14 bara, helium mass flow rate is 110 g/s, hydrogen mass flow rate is 5.2 g/s, the liquefaction rate of hydrogen is about 184 L/h. Comparison and discussion have been proposed.

The Keywords: Dynamic simulation, EcosimPro, hydrogen liquefier, helium refrigeration

1. Introduction

Hydrogen energy source as a clean and renewable energy resource will be further developed and utilized in the future. The main advantage of hydrogen as an energy carrier is the diversity in production of primary resources. Hydrogen energy can balance energy supply and demand, protect the environment and ensure energy security and economic viability [1].

Liquid hydrogen is an important source to get high purity hydrogen and ultra-pure hydrogen. Liquid hydrogen can also be used as refrigerant for high energy physics, space simulation. In addition, liquid hydrogen has unique characteristics such as lower weight and volume and higher energy content than the gaseous hydrogen. Using a hydrogen liquefier to liquefy raw hydrogen is a traditional method to get liquid hydrogen.

Production capacity of small-sized hydrogen liquefier is generally less than 20 L/h. Production capacity of medium-sized hydrogen liquefier is 20~3000 L/h. The Production capacity of large-sized hydrogen liquefier is more than 3000 L/h.

Hydrogen liquefier is a complicated multi-parameters thermodynamic system which has complex working conditions and has a high operating costs. Dynamic simulation of hydrogen liquefier improves understanding of the processes involved in hydrogen liquefier and helps in better design of the hydrogen liquefier with reduction in cool-down and warm-up time, and in the optimization of operation and controls for different system transient. In the last few years, the interest in dynamic simulations of cryogenic systems was increased significantly for the more powerful computational tools, more complex
cryogenic plants, and more require transient responses of these more complex cryogenic plants [2-4]. However, these dynamic simulation are mainly about helium refrigerators/liquefiers, the reported simulation of hydrogen liquefier are mainly about process flow. For example, Krasae-in et al. (2010) has tested efficiency of some hydrogen liquefaction process flow based on PRO/II software [5]. U. Cardella et al. (2017) have performed process optimization for large-scale hydrogen liquefaction using process modelling software UniSim Design [6]. Aasadnia et al. (2018) reviewed principle and process flow of hydrogen liquefaction and simulated simple ideal Claude cycle using Aspen HYSYS Version 9 developed by AspenONE. Aasadnia et al. (2018) believes that other simulation software, for example, EcosimPro can also be used to simulate hydrogen liquefier [7]. The dynamic simulation of hydrogen liquefiers using EcosimPro simulation software was seldom reported in recent years.

Dynamic simulations of medium-sized hydrogen liquefiers using process simulation software EcosimPro has been discussed in this research. There are two process flows, one helium turbine process flow and two helium turbines process flow. These two process flows have been discussed separately.

The paper is organized as follows: After this introduction, Section 2 gives brief introduction of software EcosimPro and cryogenic model building. Section 3 introduces dynamic simulation of one medium-sized hydrogen liquefier with one helium turbine, including process flow, dynamic simulation model, control strategy and control logic and simulation results. Section 4 introduces dynamic simulation of one medium-sized hydrogen liquefier with two helium turbines, including process flow, dynamic simulation model, control strategy and control logic and simulation results. Section 5 makes a comparison between these two simulations and ends up this paper with some conclusion.

2. Brief introduction of software EcosimPro and cryogenic model building
EcosimPro is a modelling and simulation tool for modelling 0D or 1D multidisciplinary continuous-discrete system and any kind of system based on differential-algebraic equations (DAE) and discrete events [8].

A cryogenic library named CRYOLIB has been developed and validated to simulate cryogenic systems. The source code of CRYOLIB is open which allows new properties to be easily added or modified. CRYOLIB has flexibility that the equations or correlations of the components can be also easily modified according to the actual equations are used. For most common cryogenic components modelling, such as turbine, heat exchangers, pipes, phase separator, valves and warm compressor, see [4].

The available fluids for the CRYOLIB are helium, nitrogen, hydrogen, oxygen and etc. In this research, fluids used are helium and hydrogen. Fluid properties are based on the interpolation in external tables of data generated with HEPAK (helium) and REFPROP (other fluids). HEPAK is a computer program for calculating the thermophysical properties of helium-4 (4He) from fundamental state equations and REFPROP is the NIST Reference Fluid Thermodynamic and Transport Properties Database. Users also may build their own files of fluid properties and add them to the FLUID_PROP library of EcosimPro.

3. Dynamic simulation of one medium-sized hydrogen liquefier with one helium turbine
Dynamic simulation of one medium-sized hydrogen liquefier with one helium turbine has been proposed. Process flow, dynamic simulation model, control strategy and control logic and simulation results have been discussed.

3.1. Process flow of the medium-sized hydrogen liquefier with one helium turbine
The process flow diagram of one medium-sized hydrogen liquefier with one helium turbine is shown in figure 1. This medium-sized hydrogen liquefier consists of two main parts, i.e. the helium refrigerator part and the hydrogen liquefier part. A helium refrigerator with one turbine expander provides cooling power for this hydrogen liquefier. The helium refrigeration part of this medium-sized hydrogen liquefier is a reverse Brayton cycle refrigerator, which has one helium compressor, a precooler, three heat exchangers, HEX1, HEX2 and HEX3, one helium turbine expander, one turbine inlet valve CV-2, one turbine bypass valve CV-3. The hydrogen part of this medium-sized hydrogen liquefier is mainly hydrogen source, two heat exchangers, HEX2 and HEX3 (shared with helium part), J-T valve CV-4 and one hydrogen dewar. Theoretically, there are also ortho para converters (isothermal conversion) in the hydrogen part. Its working process is: helium screw compressor discharges high pressure helium gas which flows into the cold box. Through the precooler, temperature of high pressure helium gas decreases to 80 K. Precooled helium gas expands in the helium turbine expander. The expanded helium gas flows through the heat exchanger HEX3, where cooled helium gas exchanges heat with hydrogen gas, then returns to helium compressor. Thus, a helium cycle is completed. Hydrogen part, hydrogen source gas is precooled by precooler, flows through HEX2 to exchange heat with cooled helium gas. Precooled hydrogen gas is throttled through J-T valve CV-4, then is further cooled down through HEX3. Later, the hydrogen gas liquid mixture flows into the hydrogen dewar to separate hydrogen gas with liquid. With respect to the possible two-phase flow condition in the hydrogen stream in HEX3, a dryness fraction factor will be taken into consideration when HEX3 is being designed and corresponding fluid property parameters should be taken into consideration.

The pressure ratio of helium compressor is 2/16 bara. The mass flow rate of helium gas is 111 g/s. The pressure of hydrogen source is 10 bara, mass flow rate of hydrogen gas is 4.3 g/s.

3.2. Dynamic simulator based on EcosimPro
According to process flow diagram figure 1, the dynamic simulation model of this medium-sized hydrogen liquefier based on EcosimPro is shown in figure 2. The EcosimPro version of this model is V5.0.6.
3.3. Control strategy and control logic

Control strategy and control logic of this medium-sized hydrogen liquefier with one helium turbine has been proposed.

The control logic of helium part of this hydrogen liquefier with one helium turbine is similar to the control logic of a helium refrigerator with one helium turbine [9]. The principle of control logic is to control compressor station first then to control turbine later. To stabilize compressor inlet pressure and outlet pressure first, then to connect cold box, to start the precooler simultaneously. When the inlet temperature of the second heat exchanger (high pressure side) decreases to 80 K, the inlet valve of helium turbine CV-2 will be turned on to start the helium turbine, the bypass valve CV-3 will be turned off according to the outlet temperature of helium turbine. When the outlet temperature of helium turbine decreases to 19 K, the cooling down of helium part of hydrogen liquefier is completed.

The control logic of hydrogen part of this hydrogen liquefier with one helium turbine is: to avoid too big temperature differences which hydrogen/helium heat exchangers have, hydrogen system should cool down together with helium refrigerator simultaneously.

3.4. Dynamic simulation result of this one helium turbine medium-sized hydrogen liquefier

The cooling down simulation of this one helium turbine medium-sized hydrogen liquefier has been performed. The cooling down curve of helium turbine outlet temperature is shown in figure 3. The cooling down curve of temperature T3 (in figure 1) is shown in figure 4. The liquid level curve of hydrogen dewar is shown in figure 5. The liquefaction rate is about 191 L/h.
4. Dynamic simulation of one medium-sized hydrogen liquefier with two helium turbines
Dynamic simulation of one medium-sized hydrogen liquefier with two helium turbines has been performed. The process flow, dynamic simulation model, control strategy and control logic and simulation results have been discussed.

4.1. Process flow of the medium-sized hydrogen liquefier with two helium turbines

The process flow diagram of one medium-sized hydrogen liquefier with two helium turbines is shown in figure 6. Similar to figure 1 but more complicated, this hydrogen liquefier also consists of two parts,
i.e. the helium refrigerator part and the hydrogen liquefier part. A helium refrigeration part with two helium turbines provides cooling power for this hydrogen liquefier. The helium refrigeration part is a Claude cycle refrigerator, which has one helium compressor, a precooler, five heat exchangers, two helium turbine expanders, one turbine inlet valve CV-2, one bypass valve CV-3. The hydrogen part of this hydrogen liquefier is mainly hydrogen source, three heat exchangers (shared with helium part), J-T valve CV-4 and one hydrogen dewar. Theoretically, there are also ortho para converters (isothermal conversion) in the hydrogen part.

Its working process is: helium screw compressor discharges high pressure helium gas which flows into the cold box. Through the precooler, temperature of high pressure helium gas decreases to 80 K. Precooled helium gas expands in the helium turbine expanders. The expanded helium gas flows through the heat exchanger HEX5 and HEX4, where cooled helium gas exchanges heat with hydrogen gas, then returns to helium compressor through HEX3, HEX2 and HEX1. Thus, a helium cycle is completed. Hydrogen part, hydrogen source gas is precooled by a precooler, flows through HEX2 and HEX4 to exchange heat with cooled helium gas. Precooled hydrogen gas is throttled through J-T valve CV-4, then will be further cooled down through HEX5. Later, the hydrogen gas liquid mixture flows into the hydrogen dewar to separate hydrogen gas with liquid. With respect to the two-phase flow condition in the hydrogen stream in HEX5, a dryness fraction factor will be taken into consideration when HEX5 is designed and corresponding fluid property parameters should be taken into consideration.

The pressure ratio of helium compressor is 1/14 bara. The mass flow rate of helium gas is 110 g/s. The pressure of hydrogen source is 10 bara, mass flow rate of hydrogen gas is 5.2 g/s.

4.2. Dynamic simulation model based on EcosimPro

According to process flow diagram figure 6, the dynamic simulation model of this hydrogen liquefier with two helium turbines based on EcosimPro is shown in figure 7. The EcosimPro version of this model is V5.10.2.

![Figure 7. Dynamic simulation model of hydrogen liquefier (with two helium turbines)](image)

4.3. Control strategy and control logic

Control strategy and control logic of this medium-sized hydrogen liquefier with two helium turbines has been proposed.

The control logic of helium part of this hydrogen liquefier with two helium turbines is similar to the control logic of a helium refrigerator with two helium turbines [10]. The principle of control logic is to control compressor station first then to control cold box later. To stabilize compressor inlet pressure and outlet pressure first, then to connect cold box, to start the precooler simultaneously. When the inlet temperature of the second heat exchanger HEX2 (high pressure side) decreases to 80 K, the inlet valve of the 1st helium turbine CV-2 will be turned on to start the helium turbines, the bypass valve CV-3 will be turned off according to the temperature T1. There is a relationship between the opening of CV-3 and
T1. When the outlet temperature of the 2nd helium turbine decreases to 19 K, the cooling down of helium part of hydrogen liquefier is completed.

The control logic of hydrogen part of this hydrogen liquefier with two helium turbines is: to avoid too big temperature differences which hydrogen/helium heat exchangers have, hydrogen system should cool down together with helium refrigerator simultaneously.

4.4. Simulation result of this two helium turbines medium-sized hydrogen liquefier

The cooling down simulation of this two helium turbines medium-sized hydrogen liquefier has been performed. The cooling down curve of the 2nd helium turbine outlet temperature is shown in figure 8. The cooling down curve of temperature T2 (in figure 6) is shown in figure 9. The liquid level curve of hydrogen dewar is shown in figure 10. The liquefaction rate is about 184 L/h.

![Figure 8](image8.png)

Figure 8. Cooling down curve of outlet temperature of the 2nd helium turbine

![Figure 9](image9.png)

Figure 9. Cooling down curve of temperature T2

![Figure 10](image10.png)

Figure 10. Liquid level curve of hydrogen dewar
5. Comparison and conclusion
The total UA of the hydrogen liquefier with one helium turbine is 29.9 kJ/k-s, the total UA of the hydrogen liquefier with two helium turbines is 15.2 kJ/k-s. The hydrogen liquefier with one helium turbine has a higher reliability because it has a simple structure. However, the heat exchangers of this hydrogen liquefier need bigger areas and bigger sizes. The hydrogen liquefier with two helium turbines has a more compact structure because the heat exchangers of this hydrogen liquefier need smaller areas. However, there are two helium turbine expanders in series, the system is more complicated to control.
For actual use, hydrogen liquefier with two helium turbines process flow is recommended because it is more compact.
Simulation software EcosimPro can be used to simulate hydrogen liquefier/refrigerator. However, such simulator was seldom reported in recent years. This research uses simulation software EcosimPro to simulate medium-sized hydrogen liquefiers. Two process flows of hydrogen liquefiers with one helium turbine and with two helium turbines have been simulated separately. It broadened the dynamic simulation’s applicability.

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