Transient natural gas liquefaction process comparison- dynamic heat exchanger under transient changes in flow

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Highlights:

- Two transient natural gas liquefaction processes were developed.
- Robust Model-predictive control (MPC) was designed for heat exchangers.
- Transient responses for both designs were compared.
- Natural gas consumption and liquefied natural gas production's graphs were given.

Abstract- This paper discusses transient Aspen HYSYS modeling and optimization of two natural gas liquefaction processes and identifies the rate-limiting components during load variations. The optimized model for both processes provides details for comparison. Flowrate variations included in this investigation drive transient responses of all units, especially compressors and heat exchangers. Heat exchangers commonly represent the most sensitive components to transients. This sensitivity decreases when using patent-pending dynamic heat exchanger designs and control methods. Model-predictive controls (MPC) effectively manage such heat exchangers and compare favorably with results using traditional controls. Transient efficiency graphs for both designs

illustrate improvements during model predictive control. These new controls and designs optimize natural gas (NG) consumption and liquefied natural gas (LNG) production.

Keywords: natural gas liquefaction, transient modeling, optimization, Aspen HYSYS

1. Introduction

Recently promulgated EPA regulations under Clean Air Act Sections 111(b) and 111(d) aggressively limit CO₂ emissions from the US power industry. [1]. Under these regulations, new natural-gas- and coal-fired power plants can emit up to 500 and 635 kg of CO₂ per MWh. CO₂ emissions reductions from existing plants require about a 32% overall reduction from 2005 levels, although the regulation is not written in this way. The standard requires states or groups of states to meet specified total emission targets or, as an alternative, to meet emission rate targets. Current combined-cycle natural gas plants meet the standards for new power plants as they are about 50% below the emissions of most coal plants. Nevertheless, the regulation has specific provisions for limiting the amount of natural gas used to meet the new standards for existing power plants. Such large reductions from coal plants lie well beyond the reach of plant efficiency improvements or other modest operational changes and threaten decommissioning of existing plants and curtailing plans for new plants. In fact, coal consumption has declined in the US and in parts of Europe for several years and there are very few new coal plants planned.

The recent declines in coal consumption in the US largely result from low-cost natural gas competition and not from CO₂ emissions controls. Globally, fossil fuels in general and coal in particular are the most rapidly increasing primary energy sources [2]. Projected future energy sources show coal and other fossil fuels will continue to play major roles in power generation in the US and globally [3]. Power generation accounts for about one-third of the total CO₂ emissions

in the US and globally [4, 5]. Global CO₂ emissions must decrease by 52-70% from 2012 levels by 2050 to limit global climate change to a 2 °C increase [6]. This required reduction in total CO₂ emissions represents about twice as much CO₂ as that emitted from all forms of power generation in 2012, even without including future increases emissions. Therefore, global climate change mitigation requires eliminating about twice as much CO₂ as all current emissions from power generation. Emissions from power generation are large, stationary, and generally continuous sources and should be far less expensive to curtail than mobile sources or distributed, intermittent, small sources such as retail and residences. Successful climate-change mitigation critically depends on finding ways to reduce CO₂ emissions from fossil power plants. No national or global climate change policy can likely succeed without developing and deploying some kind of carbon capture technology.

Climate change mitigation also depends on increased deployment of renewable energy, especially wind and solar. Renewable energy has many redeeming virtues, but its intermittency is a major barrier to effective and reliable contributions to the grid. Arguably, the greatest technical need to increased effectiveness of renewable energy is affordable, efficient, utility-scale, rapidly responding energy storage. Energy-storing Cryogenic Carbon Capture™ (CCC) is a potential solution to both the carbon capture and the energy storage challenges in climate change mitigation.

Various methods of commercial-scale CO₂ capture promise to improve the environmental-friendliness of coal-fired power production [7-9]. Cryogenic Carbon Capture™ (CCC) is a post-combustion, retrofit or greenfield technology [10] that reduces carbon emissions from fossil-fueled power plants by 95–99% at half the cost and energy demand of current state-of-the-art carbon capture processes while providing efficient, rapidly responding, grid-scale energy storage [11,12] (Figure 1). In addition, CCC removes other pollutants, such as SO_x, NO_x, PM_{xx} and mercury. CCC

desublimates CO₂ and condenses or desublimates other pollutants, removing all species less volatile than CO. Capture efficiency increases as temperature decreases. At low enough temperatures, the exhaust exiting the stack could contain less CO₂ than the ambient air [12, 13]. The external cooling loop configuration (CCC ECL) also provides significant energy storage and is the focus of this paper.

CCC ECL consists of two major subsystems: cryogenic carbon capture [12], and energy storage via natural gas liquefaction [14]. Natural gas liquefaction provides refrigerant for the CCC process [14].

The CCC process (1) dries and cools flue gas, (2) further cools the flue gas in a heat recovery heat exchanger to nominally -107 °C, (3) condenses contaminants such as mercury, SO₂, NO₂, Hg, and HCl at various stages during cooling (cooling happens in stages even though it is illustrated in a single step), (4) separates the solid CO₂ that forms during cooling from the remaining gas, (5) pressurizes the solid CO₂ to 70-80 bar, (6) reheats the CO₂ and the remaining flue gas to near ambient conditions (15-20 °C) by cooling the incoming gases, and (7) compresses the pressurized and now melted CO₂ stream to final delivery pressure (nominally 150 bar). Most of these steps involve traditional industrial processes; however, cooling the gas efficiently while de-sublimating CO₂ required innovation of new, patented desublimating heat exchangers [15, 16]. Figure 2 illustrates the major process steps without the energy storage component.

The CCC process operates with the same amount of refrigerant generation and use in normal operation or balanced mode. The energy-storing (ES) mode of the process generates more refrigerant than the carbon capture process uses and stores the excess refrigerant in an insulated vessel as a liquid at the low-temperature, modest-pressure point in the cycle. This normally occurs

during off-peak hours or when excess power from wind farms or other intermittent sources enters the grid. During peak demand, the stored, condensed refrigerant provides energy recovery (ER) by reducing the compressor load, decreasing the energy required to operate the cryogenic carbon capture and delivering the saved parasitic load to the grid for as long as the stored refrigerant lasts. The amount of refrigerant required by CCC for 3-4 hours of utility-scale power plants requires only a fraction of the capacity of commercially available LNG storage tanks.

Figure 3 illustrates the overall energy storing process. The straight line is the constant energy stream needed to capture CO₂ from a plant operating at constant load. The net plant output meets the varying demand, as indicated by the red line. The yellow line represents the NG flow into the plant. The difference between the yellow line and the average demand would be the net NG outflow either into a simple cycle turbine or the NG pipeline. This investigation focuses on the LNG generation process during the transients in NG flow.

Liquefaction systems generally comprise a series of compressors, coolers, expanders, and heat exchangers. Well-designed Heat Exchanger Networks (HENs) can significantly contribute to a decrease in energy consumption and, therefore, energy expenses [18-20]. With proper design of natural gas liquefaction, the CCC process allows the energy demand to occur when power costs are low and availability is high. This time shifting or demand response enables a form of energy storage at very large scale that is highly efficient and very cost effective. This allows a fossil plant to follow load and to absorb intermittent renewable contributions at arbitrary times, effectively shifting the renewables and low-cost, low-demand power periods to peak demand times. This potentially continually transient liquefaction process could suffer inefficiencies and high maintenance costs associated with transient and large differences in stream temperatures in the heat exchangers if not properly managed. Mixed refrigerant (MR) cycles are effective in reducing

the temperature difference [21], but flowrate changes can undo an otherwise well designed refrigerant system. This investigation focuses on details of heat exchanger performance and managing these flowrate changes. Previous work examines the grid-level energy storage contributions and the substantial economic benefits of this process [7, 8, 13]. The CCC process described here could be the most strategically important technology for both fossil and renewable energies.

Most NG liquefaction investigations focus on steady-state operation [22-26]. Although there are many publications on the steady-state design and optimization of LNG processes, there are only a few transient models. A dynamic process simulator predicts transients, dynamics, and control scheme behavior. The turbo machinery and most portions other than heat exchangers adapt relatively easily to the transients. The heat exchangers, however, become significantly imbalanced during these transients, leading to large thermal stresses and inefficiencies associated with large local changes in temperature and temperature differences. These imbalances prematurely age equipment and cause the process to miss specifications and perhaps fail completely. Using dynamic simulation, this investigation evaluates design modifications and capture cases and quantifies the effects of flowrate changes on efficiency and other process figures of merit.

This investigation models transient natural gas liquefaction in two ways using Aspen HYSYS Dynamics: traditional heat exchanger design (THED) and dynamic heat exchanger design (DHED). In THED, Aspen HYSYS dynamics optimizes a single mixed refrigerant (SMR) process. In DHED, patent-pending dynamic heat exchangers use two methanol streams in addition to the traditional streams to regulate flow rate and heat exchanger temperature profiles during transients [17, 27]. Operating conditions, MR compositions and the nominal heat exchanger size remain the same for both designs. K-value and U-value techniques manage heat exchanger flow rates and

temperature profiles. All cases involve LNG and NG transients. Heat exchanger temperature profiles and efficiency depend on operating conditions, as discussed below.

2. Process design

2.1. Feed gas parameters

The simulations discussed in this paper require several specifications, as summarized in Table 2. A feed gas flow rate of 21200 kgmol/h represents the amount of natural gas required for the steady operation of CCC on a 550 MW power plant. During energy storage and recovery, the rates change to 29680 kgmol/h and 6360 kgmol/h, respectively. These flow rates represent a 40% increase and a 70% decrease in coolant flow. The assumption here is that the amount of cooling the LNG provides to the CCC process remains constant (constant boiler load) while the demand on power for the LNG production process could change +40% to – 70% based on grid variations. In reality, the off-peak period commonly lasts much longer than the peak period, but this simple approach illustrates how the system works and is a worst-case scenario from a controls standpoint. All other parameters mentioned in Table 3 remain constant. The liquefaction rate is 100% after the main heat exchanger, but to satisfy the CCC process, that is, to avoid temperature cross in CCC's heat exchanger, the output temperature from the LNG plant should be around -120 °C. Therefore, LNG partially vaporizes (27%) after the main heat exchanger.

2.2. Liquefaction process- Single Mixed Refrigerant cycle (SMR)

The single mixed refrigerant (SMR) is the simplest NG liquefaction process and in previous analyses is the most efficient [14]. The SMR cycle uses only one MR loop for pre-cooling, liquefaction, and sub-cooling (Figure 4). The cycle compresses and cools the refrigerant until liquid forms, and then vaporizes the refrigerant in the LNG exchanger. The refrigerant cools and

condenses the natural gas, NG, to liquefied natural gas, LNG. The refrigerant composition generates net warm- and net cold-stream temperature profiles in the heat exchangers that are close and parallel, though nonlinear.

A single LNG heat exchanger liquefies and cools the natural gas to the required LNG storage condition of about -119.4 °C and 11.45 bar pressure. Subsequent expansion prepares the LNG for the CCC process. The LNG can optionally cool further and be stored at lower pressure, with less evaporation prior to entering the CCC process, but the conditions here provide a sufficient basis to illustrate the dynamic responses of the system. The return natural gas (now all vapor) stream and a stream of water condensed from the flue gas return from the CCC process to the LNG process. Water reduces heat load. Table 4 summarizes the optimized mixed refrigerant composition and key parameters, where ER, B and ES represent energy storing, balanced, and energy recovery respectively.

There are two dynamic heat exchanger configurations. The first configuration involves the THED process shown in Figure 4a and the second configuration introduces two additional methanol streams, as shown in Figure 4b. In practice, these two streams could be a single pipeline, but pipelines can flow in both directions confuse the simulation software. The dynamic heat exchangers are patented innovations that maintain internal heat exchanger temperature profiles near their balanced condition by filling or emptying the storage tanks during an operational transient, using the flow rate difference to change the relative flow rates in the heat exchanger [18, 27]. The system manages transients by either filling or emptying a tank. These dynamic heat exchangers benefit the process in several ways. In their absence, natural gas flow rate changes create temperature profile changes in the heat exchanger. PID controllers try to compensate by adjusting refrigerant flow rate, but refrigerant flow rate changes alone cannot completely restore

the optimized temperature profile. Large temperature changes in the heat exchanger cause thermal stresses as well as efficiency losses. The dynamic system can solve these issues. If an upset or transient changes one of the cold or hot flows, the dynamic system compensates by adjusting the balancing stream through filling one tank by emptying the other tank such that the heat exchanger functions at its highest efficiency. A future transient or upset in the opposite direction allows the system to return to its baseline condition, including the original levels of stored material in the tank. Therefore, the system levels the periodic changes in flow, random transients, and other dynamics. The dynamic systems cannot fully compensate for a permanent shift in flow rates, but they can nearly perfectly compensate for temporary changes around some average and they can spread the transition to a long-term change over a long enough time to avoid unallowable thermal stresses and set point errors.

The dynamic heat exchangers in this configuration can use essentially any fluid in the channels that connect the two tanks. An ideal fluid has minimal safety issues and a low melting point, a high boiling point, and a high volumetric heat capacity. That is, it should be a liquid with the ability to absorb as much heat as possible with minimal change in temperature. These simulations use methanol. The Peng-Robinson (PR) equation of state provides most of the thermodynamic VLE basis in this simulation [28].

3. Results and discussion

3.1. Process optimization

This optimization is a non-automated version of the genetic algorithm. Several variables appear in the optimization objective function for the mixed refrigerant stream including pressure, composition, and flow rate along with the pressure exiting the expansion turbine. The algorithm

205 changes multiple parameters including pressure, composition, and flow rate of the mixed
206 refrigerant stream as well as the exit pressure of the turbine. The individual components of the
207 mixed refrigerant stream, C1-C5 n- hydrocarbons, varied instead of composition and overall flow-
208 rate. This reduces the number of optimization parameters to seven. All of these parameters vary
209 continuously and there is no reason to expect that any of them generate discontinuities in either
210 the objective function or its partial derivatives. Each variable had three to five values specified,
211 including mid-, low-, and high-values. The decision to include additional higher and/or lower
212 values depends on the previous set of variables. Aspen's sensitivity analysis tool calculates the
213 total power required by the cooling loop and the conditions that led to that result. A subset of the
214 best solutions combines pairwise to form a set of new input test values through cross-over or
215 recombination algorithms, which are generally linear combinations of the parameters of the parent
216 solutions. Many algorithms also employ mutation searches in which one or more new parameters
217 assumes values that differ from genetic or linear combinations of the previous solutions. No
218 mutation searches appeared necessary in this problem. The process repeats until the optimal
219 solution repeats several times with adjustments to input values. The specific algorithm tuning
220 parameters (weighting of properties of the parents in creating new parameter sets, probabilities of
221 parents being selected and paired, and conditions for defining optimum) affected the time required
222 to find the optimum but did not lead to different optima. These optimal conditions appeared to be
223 robust with respect to initial conditions and optimization tuning parameters and this investigation
224 did not explore further details of varying parameters in this algorithm. Genetic algorithms have
225 advantages for objective functions that are discontinuous, non-differentiable, stochastic, or highly
226 nonlinear or that have multiple local minima. The objective functions used here should be
227 continuous, deterministic, and in principle differentiable. However, they can be highly nonlinear

and may have multiple local minima. The process minimizes the work done per unit of LNG production (the objective function):

$$f(X) = \min \left(\frac{W_{net}}{q_{LNG}} \right) \quad (1)$$

Where

$$W_{net} = \sum W_{compressor} - \sum W_{expander} \quad (2)$$

and q_{LNG} represents the mass flow of the produced LNG.

The model assumes:

- 1) A minimum of 1K approach temperature in brazed plate heat exchangers [12,14,17,18, 27,29-31]
- 2) Compressors operate at 92% isentropic efficiencies with no condensates,
- 3) Inter- and after-coolers are capable of cooling the gases to 20 °C
- 4) A single liquid phase in turbines and pumps (100% liquid flow)
- 5) Expansion valves operate adiabatically.

Some of these assumptions may not be achievable in practical systems, and others have detailed the consequences of relaxing them on the overall energy and cost performance of the CCC system [11]. The present analysis explores the transient behavior and these behaviors are most critical under these aggressive conditions. THED optimization proceeds as explained above. The DHED uses all the optimized conditions from THED. In addition, it optimizes two methanol streams'

conditions to obtain optimum pressure, temperatures and flow rates. Methanol thermodynamic properties determine the temperatures and pressures. The following discussion outlines the details of this optimization.

Model-predictive control (MPC) provides the heat exchanger control for this model. MPC requires solutions at multiple natural gas flow rates. A base case determines a baseline heat exchanger ΔT by an enthalpy balance on both sides of the heat exchanger. Mixed refrigerant and methanol flow rates restore the baseline ΔT during optimization.

Generally, optimization would follow this procedure for many natural gas flow rates. Visual Basic for Application (VBA) code in Excel saves time and simplifies the process. The code first links VBA to HYSYS. Once it links, VBA calculates the current ΔT of the heat exchanger and the difference in the ΔT 's of the heat exchanger using the base case as a reference. The built-in Excel solver minimizes the difference in ΔT 's by changing the mixed refrigerant and methanol flow rates. Once it converges, it records the flow rates needed to converge and then it changes the natural gas flow rate to a new value and then iterates the entire process.

These data provide a list of methanol flow rates versus natural gas flow rate. Empirical equations fit the data for the mixed refrigerant and methanol flow rates. Aspen verifies the validity of these empirical results and the validated correlations accelerate the optimization procedure by avoiding lengthy Aspen calculations.

Energy input requirements for both THED and DHED are given in Table 5 that indicates that DHED requires less energy compared to THED in both the energy recovery and energy storage modes and only slightly more energy in the balanced mode. The next section describes heat

exchanger efficiency, followed by a discussion of the slight increase in the balanced mode. On average, the DHED system requires significantly less energy than the THED mode.

3.2. Heat exchanger efficiency

This document defines a heat exchanger efficiency that forms a figure of merit for heat exchanger performance. Insulated heat exchangers conserve enthalpy, so a first-law definition is problematic. That is, the enthalpy flowing out of the system equals that flowing in. Heat exchangers do not involve shaft work, so a second-law definition (work over heat) does not naturally come to mind. Nevertheless, this document proposes a second-law definition for heat exchanger efficiency that is both useful and simple [18].

Conceptually, this efficiency describes the consequence of heat exchange on the flow streams' (a) ability to do work (availability or exergy) or, equivalently, (b) entropy production. Quantitatively, the heat exchanger efficiency is one minus the difference in exergy between the streams exiting and entering a heat exchanger normalized by the largest achievable difference in such exergy. The largest achievable difference with respect to heat exchange occurs if all the streams come to the same temperature. These analyses and this definition assume no heat transfer between the exchanger and its surroundings. Therefore, the difference in exergy is proportional to a difference in entropy, with the ambient or heat rejection temperature as a proportionality constant. This expression depends on conditions at thermal equilibrium, that is, at the temperature the streams would become if the inlet streams were to equilibrate at a single temperature

$$\eta = 1 - \frac{\sum_{outlet} m_i \hat{b}_i - \sum_{inlet} m_i \hat{b}_i}{\sum_{eq} m_i \hat{b}_i - \sum_{inlet} m_i \hat{b}_i} = 1 - \frac{\Delta_{obs} m_i \hat{s}_i}{\Delta_{eq} m_i \hat{s}_i} = \frac{\sum_{eq} m_i \hat{s}_i - \sum_{outlet} m_i \hat{s}_i}{\sum_{eq} m_i \hat{s}_i - \sum_{inlet} m_i \hat{s}_i} \quad (3)$$

where $\hat{b}_i = \hat{h}_i - T_0 \hat{s}_i$ represents the specific exergy of stream i and $\Delta_{eq} m_i \hat{s}_i$ is the difference between the entropy in all the streams at equilibrium temperature and entropy of the streams at the inlet temperature. The temperature T_0 represents the temperature of the ambient or heat rejection environment and, since it drops out of the equation, is irrelevant to the exchanger efficiency. This ambient temperature should not affect a well-posed efficiency definition for reasons discussed below. The middle form of the equation results from the sum of the inlet enthalpy flows equaling the sum of the outlet enthalpy flows.

This investigation makes frequent reference to this efficiency in the context of functioning processes. Nonfunctioning processes can lead to results that illustrate a distinction between efficiency and effectiveness. The efficiency by this definition would be unity in the extreme case of a completely dysfunctional exchanger that transfers no heat among streams. However, the effectiveness would in this case would be zero.

This efficiency becomes unity if the total exergy of the outlet streams equals that of the inlet streams, which can only occur in the limit of the hot and cold streams transferring heat with no temperature difference at any given point along the exchanger (ideal heat exchanger). The efficiency is zero if all outlet streams approach the same equilibrium temperature, which represents the poorest possible heat exchanger performance from an efficiency or entropy standpoint. An efficiency of 50% indicates that the heat exchanger generates half of much entropy as it would generate if all streams come to the same temperature. Heat exchanger's efficiencies in steady state for both THED and DHED appear in Table 6.

Table 6 indicates DHED efficiencies differ only slightly among the balanced, energy recovery, and energy storing modes. The two-tank system leads to a stable efficiency that is close to the

balanced case in DHED. This investigation shows that DHED heat exchanger efficiencies are on average higher and more constant compared to THED, as discussed shortly. In DHED, the heat exchanger temperature profiles are the same in all three cases (storing, recovery, and balanced), eliminating thermal stress and minimizing the required size of the heat exchangers.

The reason for the slightly higher energy requirement and slightly lower efficiency of the DHED system compared to the THED system in balanced mode is that the heat exchanger total surface area (and therefore cost) are the same in both systems. However, the DHED system includes two additional streams in the heat exchanger that, in balanced mode, will have a flowrate of zero. Therefore, these stagnant streams decrease overall efficiency with a commensurate increase in energy demand in balanced mode. In all other modes, these streams more than compensate for the compromise in balanced mode. These differences in efficiency and energy demand would decrease with increasing heat exchanger surface area to compensate for the effect of the stagnant stream. This investigation chooses not to do this to illustrate the advantage of the DHED process for transient flows. That is, larger heat exchangers can always decrease energy demand somewhat, but in the case of transient flows, the DHED system can save energy even though it slightly compromises the balanced behavior. A second version of the dynamic heat exchanger, the retrofit version, could eliminate the disadvantage of the configuration shown here in balanced mode and actually slightly improve on the performance in energy storing and energy recovery mode, but it is not well suited to heat exchangers with gaseous streams [18, 27].

3.3. Transient modeling

3.3.1. Dynamic heat exchanger modeling

Accurate equipment sizing, proper pressure or flow rate specifications as boundary conditions and specifying resistance of unit operations all factor into the dynamic simulation of the plant. Geometry information is important since transient behaviors depend on equipment size. Rating of a multi-stream, brazed plate heat exchangers includes:

- a) Length and width of the exchanger
- b) Layer configuration
- c) Zone configuration
- d) Heat transfer configuration.

3.3.1.1. Length and width of the heat exchanger

Aspen economic analysis in HYSYS estimates total surface area which is divided among each zone and each layer.

3.3.1.2. Layer configuration

Stream setup affects the total heat load distribution. Optimal layer configuration assumes single banking of cold and hot layers with countercurrent flow on the dynamic tab. Specified inlet and outlet streams' zone and layers in zone zero cascade through all twenty zones in these simulations.

3.3.1.3. Zone configuration

In a pressure-flow solver dynamic model, heat exchanger calculates flowrates using resistance equations. Each zone features a stacking pattern with one feed and one product connected to each representative layer in the pattern. Resistance equation modeled after turbulent flow equation is:

$$F = k\sqrt{\rho \times \Delta P} \quad (4)$$

352 Where:

353 k = pressure flow coefficient, $\frac{kg}{h} \times \sqrt{\frac{\frac{kg}{m^3}}{kPa}}$

354 ρ = density of fluid, $\frac{kg}{m^3}$

355 ΔP = total pressure drop, kPa

356 The resistance equation calculates flowrates from the pressure differences of the surrounding
357 nodes using pre-specified k-values. Dynamic heat exchangers require k-values. However,
358 temperature and pressure drops for each zone are not known a priori; thus, exact k-values cannot
359 be specified. Specified temperature and pressure drops on the dynamic tab allow the process to
360 calculate K's. K-value set up is one of the most important steps for heat exchangers' design in
361 dynamic mode and errors in this step might lead to pressure and temperature imbalances and even
362 reverse flows during the transient estimates.

363

364 3.3.1.4 Heat transfer configuration

365 The global heat transfer coefficient, UA, calculates the convective heat transfer between the steam
366 and the metal that surrounds it. Aspen HYSYS provides UA values for each stream; hence, surface
367 area determines U for each layer. Aspen Economic Analysis sizes and costs the equipment,
368 including heat exchangers' surface area (A). Equal UA-values remain constant for a layer in each
369 zone. Steady state UA values provide initial estimates.

These steps are the same for both THED and DHED, but since the DHED balanced case includes two zero flow rates in the methanol streams and, for ER and ES cases, one methanol stream zero flow rate, proper K values and U values are important. Both THED and DHED use the same sizing. The highest flow rates use K-values and the balanced case uses U-values. Aspen HYSYS automatically scales these K values and U values with respect to flow rates passing through each stream.

3.4. Transient modeling of natural gas liquefaction process

Aspen HYSYS provides dynamic simulation of this process. The following features make the process efficient and effective in transient mode, including:

- 1) Changing mixed refrigerant flow rates in THED control the output temperature through a PID controller.
- 2) Digital on/off controllers regulate cooling water flow rate. Specifically, when natural gas flow rate is below its average value, the water flow turns on and when the natural gas is above its average, water flow turns off.
- 3) Transfer functions have two important impacts. One breaks the closed loop, which greatly increases the convergence speed. Transfer functions force the input of an open loop to equal the output, making an open loop function like a closed loop. Transfer functions also provide the values of the ramping flow rates in the simulation. Both step changes and ramping flow rates illustrate the dynamic responses. During a step change, flow rates of natural gas change with three specific flow rates. Figures 5a, 5b, 6a and 6b illustrate transient changes in total energy use, NG turbine production, MR turbine production and NG flow rate for the THED. Figures 7a, 7b, 8a and 8b illustrate similar performance for the DHED system. Changing NG flow rate also changes total energy usage since the

compressors' energy demand changes. Figures 5-8, indicate how the DHED compares to THED during flow rate variation.

- 4) Heat exchanger temperature profiles provide some of the most important information on efficiency and effectiveness. The temperature profiles for THED can be found elsewhere [17].

One of the most important goals for DHED is to have one temperature profile for all three cases. Figure 9 illustrates this constant temperature profile. The temperature difference and heat exchange load contribute to the exergy loss. If the hot composite curve matches the cold curve well, the resulting exergy loss is small.

These results lead to several observations

- a) Transient models require some process changes.
- b) The two methanol streams have zero flow rates in balanced case but for ER and ES flow rates have been optimized using MPC.
- c) As natural gas flow rate changes, there is no change in temperature in the heat exchanger for DHED. Also the efficiency does not appreciably change. By contrast, the THED temperature profiles and efficiency change markedly with changing flows.
- d) All units in HYSYS include dynamic responses. For example, coolers and heaters maintain specified product temperatures. The coolers use water and the heaters use steam.
- e) The turbomachinery has constant efficiencies and pressure changes regardless of the flow rate in this model. Measured efficiency and pressure curves are reasonably flat over wide ranges, but they are not entirely constant.

3.5. Transient efficiency

The transient spikes seen in THED data virtually disappear under DHED. Even though the process goes through a relatively large transient – the same transient indicated in Figure 10a – the heat exchanger maintains nearly constant conditions. This reduces energy input requirements for the whole system and exergy losses for the heat exchangers. The efficiency for DHED exceeds that of the THED as shown in Figure 10 where DHED efficiencies are higher and constant, even during transients.

3.6. Rapid system response

In addition to maintaining optimal efficiency and meeting set points through transients, this innovation allows the system to move much more rapidly through these transients. This is a significant benefit to several processes. Unlike THED, which experience thermal stresses and other temperature-profile-related performance concerns through transients, DHED has no such issues. This allows the process to move through transients, change loads, and follow set points at much more rapid speeds than is otherwise the case. One important comparison would be comparing LNG production and NG consumption for two models. For THED with manually tuned PID controller, it usually takes 10-20 minutes for THED with perfectly auto tuned PID controller to adjust to the new conditions. By contrast, it takes 2-7 minutes and for DHED to adjust. As these figures (Figures 11a, 11b and 11c) indicate, the DHED process is more stable. All units including compressors, heat exchangers and expanders are more adjustable to transitions compared to THED.

4. Conclusions

Aspen HYSYS simulations of two natural gas liquefaction processes that provide coolant for the energy-storing version of the CCC indicate process performance in transient modes. During energy storage, energy demand increases significantly since excess LNG is produced. During energy recovery, the energy demand decreases since stored LNG supplements the amount produced from the process. The two processes differ in the construction of heat exchangers, one being a traditional LNG design and the second being an innovative new dynamic heat exchanger design. Heat exchanger performance based on efficiency and energy demand illustrates that the dynamic heat exchangers are more efficient and demand less energy on average but under balanced conditions are slightly less efficient and demand slightly more energy. The balanced behavior could be made equally efficient if the heat exchanger size increases, but this analysis compared to comparably sized heat exchangers. The discussion highlights transient modeling techniques including K-values, U-values, zone configuration and heat transfer rating. The discussion includes transient efficiency, flow rate, temperature profile, and other characteristic graphs for both designs. All of the results are optimized within the constraints of the system.

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Figure 1 Projected forts year costs and parasitic of CCC with various integration in a Greenfield installation [11]

Figure 2 Cryogenic Carbon Capture Flow Diagram

Figure 3 Typical power plant and system demand patterns in three cases [17]

a)

b)

Figure 4 Aspen HYSYS simulation of SMR for a) THED b) DHED

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Figure 5 Ramping a) B-ER-B performance b) B-ES-B performance [17]

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Figure 6 Step changing a) B-ER-B performance and b) B-ES-B performance [17]

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b)

Figure 7 Ramping a) B-ER-B performance and b) B-ES-B performance

a)

b)

Figure 8 Step changing a) B-ER-B performance and b) B-ES-B performance

Figure 9 Temperature profile for DHED

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a)

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b)

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c)

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Figure 10 Transient efficiencies for a) THED and b) DHED with respect to MR and c) NG flow rates

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a)

b)

c)

Figure 11 LNG (solid red line), kgmol/h; NG (solid black line), kgmol/h; a) THED with manually tuned PID controller b) THED with perfectly auto tuned PID controller and c) for DHED

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Table 1 Common Pollutant Removal Temperatures

Temperature (°C)	What is captured
-48	100% of the mercury in coal
-77	All of the above, plus 99% of the mercury from the atmosphere
-117	All of the above, plus 90% of the CO ₂ from coal; SO ₂ EPA standard met
-132	All of the above, plus 99% of the CO ₂ from coal
-143	All of the above, plus 100% of the CO ₂ from coal. Below this point, the exhaust exiting the stack is cleaner than the surrounding air.
-150	All of the above, plus 80% of the CO ₂ from the atmosphere
-162	All of the above, plus 99.5% of the CO ₂ from the atmosphere

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Table 2 Mole fractions of the feed gas and other parameters in the process

Parameters	Value	Notes
Feed gas pressure	3700 kPa	
Feed gas temperature	21 °C	
Feed gas flow rate	21200 kgmol/h	
Feed gas mole fraction components	CH ₄	0.95
	C ₂ H ₆	0.03
	C ₃ H ₈	0.02
LNG storage pressure	1145 kPa	
LNG temperature before expansion	-94 °C	
Liquefaction rate before expansion	100%	
NG temperature after expansion	-119.4 °C	
Liquefaction rate after expansion	73%	

Pressure drop in heat exchanger	5 kPa	To simplify the process
Pressure drop in water cooler	1 kPa	
Temperature after water cooler	21 °C	
Ambient temperature	25 °C	
The adiabatic efficiency of compressor	92%	[12,14]
The adiabatic efficiency of turbine	92%	[12,14]
Pressure ratio of each compressor	1-3	
Water's temperature from CCC	1.0561 °C	
From CCC's temperature	-98.5 °C	
The minimum approach temperature of heat exchanger	1-3 °C	

Table 3 Basic condition for all four models

Conditions	From pipeline	To CCC (final conditions)
Vapor / Phase Fraction	1	0.27
Temperature [C]	21	-119.4
Pressure [kPa]	3700	1145

Table 4 Mixed refrigerant conditions and key parameters for three cases

Entrance				Loop		
Conditions	ER	B	ES	ER	B	ES

Vapor / Phase	0.43	0.023	0.00	0.23	0.086	0.10
Fraction						
Temperature	30.00	20.5	16.12	-87.99	-93.191	-92.05
[C]						
Pressure [kPa]	3704.65	3704.65	3704.65	108.4	108.394	108.40

Component	Mole fraction
Methane	0.0418
Ethane	0.8461
Propane	0.0017
n-Butane	0.0053
n-Pentane	0.1051

Table 5 Optimized energy input requirements in DHED for each case

Energy input requirements	ER (kW/kg NG)	B (kW/kg NG)	ES (kW/kg NG)
THED	0.00831	0.06126	0.07065
DHED	0.00486	0.06132	0.05092

Table 6 Heat exchanger's efficiency in DHED each case

Heat exchanger's efficiency	ER (%)	B (%)	ES (%)
THED	74.35	93.86	80.21
DHED	91.43	91.92	91.80