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Heat exchanger simulations involving phase changes

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1. Introduction

There are probably more heat exchangers in most chemical and petroleum plants than any other type of unit, excluding pumps and piping. Process streams must be heated or cooled by using utilities or process streams at higher or lower temperatures. High energy costs have increased the economic incentives for investing in heat-transfer area in order to reduce energy requirements for both heating and refrigeration.

At the conceptual design stage of a project, the typical approach is to use heuristic values for overall heat-transfer coefficients (*U*) that are suitable for conditions on the hot and cold sides of the heat exchanger. Systems with gas phases on both the hot and cold sides have small *U* values. Turton et al. (2003) suggest $0.17 \text{ kW m}^{-2} \text{ K}^{-1}$. Systems with gas on one side and condensing vapor or boiling liquid on the other side have higher *U* values ($0.28 \text{ kW m}^{-2} \text{ K}^{-1}$). Systems with liquid on one side and condensing vapor or boiling liquid on the other side have even higher *U* values ($0.85 \text{ kW m}^{-2} \text{ K}^{-1}$). Systems with liquid phases on both sides have *U* values around $0.57 \text{ kW m}^{-2} \text{ K}^{-1}$.

These values are typical for processes with reasonable fluid velocities, which are achieved by designing flow areas to give reasonable pressure drops. One of the important engineering trade-offs is balancing capital investment in heat-exchanger area against energy costs for pumping and compressing. The main reason for the low *U* values in gas-gas systems is the high cost of compression in

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ABSTRACT

Heat exchangers in which phase changes occur are widely applied in industry. Condensing vapor streams and boiling liquid streams are important components in almost all flowsheets of chemical processes. The accurate modeling of these systems is important at the design stage so that heat exchangers with adequate heat-transfer area are purchased and installed.

The purpose of this paper is to illustrate that some caution must be exercised in developing simulation models for heat exchangers when liquid is vaporized or vapor is condensed. Use of simple standard heat exchanger models can lead to incorrect differential temperature driving forces and gross underestimation of heat-transfer area.

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order to provide pressure drop through heat exchangers (adequate fluid velocity).

The capital investment in heat exchangers is normally a very significant fraction of the total plant investment. For example, the capital costs of the reboiler and condenser in a typical distillation column are about the same as the capital cost of the vessel.

Accurate modeling of heat-exchanger performance is clearly of great significance. The cost of having to retrofit additional heat-transfer area after the plant has been built can be an order of magnitude more expensive than the cost when part of the original design. Lost production is usually much more costly.

The modeling of heat exchangers in which no phase change occurs is fairly straightforward and relatively free of dangerous pitfalls. The same cannot be said for modeling of heat exchangers in which gases are condensed and/or liquids are vaporized. This paper discusses some of the issues and potential poor predictions of required heat-transfer areas. The widely used Aspen Plus software illustrates some of the problems. Peng–Robinson physical properties are used.

2. Process studied

As a typical example, we consider a low-level energy recovery process with a working fluid (n-hexane) that is circulated around through the system. Liquid hexane is pump to a high pressure and vaporized in a heat exchanger (evaporator). The heating source is hot air at 90 °C, which is saturated with water. The vapor is expanded through a turbine to generate power and condensed in a second heat exchanger using cooling water at 25 °C. A pressure–enthalpy diagram for the working fluid n-hexane given in



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Fig. 1. n-Hexane PH diagram.

Weber (1956) is shown in Fig. 1. Fig. 2 gives its vapor pressure curve over the range of temperatures of interest in this process (source at 90 °C and sink at 25 °C).

The energy source is 50 kg/s of hot air (90 °C and 1 bar) that is saturated with water. It is fed into an evaporator in which liquid n-hexane boils at a pressure of 1.25 bar (corresponding to the saturation temperature of 75.5 °C for the pure component). The flowrate of the working fluid hexane is 90 kg/s. The gas is expanded through a turbine to 0.273 bar (corresponding to the saturation temperature of 31.1 °C in the downstream condenser). The power generated is 3.5 MW. The hot gas (air and water) cools as it flows through the evaporator, and there is some condensation of liquid water in the gas stream. This greatly increases the overall heat-transfer coefficient in the evaporator since there is vaporizing liquid hexane on the cold side and condensing vapor water on the hot side. An overall heat-transfer coefficient of 1.4 kW m⁻² K⁻¹ is assumed.

The conditions presented above were determined from an economic optimization study to find the maximum return on



Fig. 2. n-Hexane vapor pressure.

investment. The credit is turbine power. The capital investment is in two heat exchangers, turbine and pump. The design optimization variables used are evaporator pressure, condenser pressure and working fluid flowrate. Heat-exchanger area in the evaporator increases as evaporator pressure *increases* (smaller differential temperature), but turbine power increases (larger expansion ratio). The opposite effect occurs in the condenser. Heat-exchanger area in the condenser increases as condenser pressure *decreases* (small differential temperature), but turbine power increases (larger expansion ratio).

Increasing the flowrate of the working fluid generates more power in the turbine but increases heat-transfer areas in both the evaporator and condenser since higher heat-transfer rates are needed to vaporize and condense the larger flow of hexane.

A series of cases were run exploring the three-dimensional space of the three design variable to find the conditions that give the maximum return on investment. At the pressures and hexane flowrate given above, the total capital investment is \$8,436,000 with the turbine (\$1,192,000), evaporator (\$1,494,000) and condenser (\$3,251,000) being the major capital cost items. The value of the turbine power is \$1,866,000 per year (assuming a \$16.8 per GJ value), giving a 17% return on investment.

3. Simple heat exchanger simulation

The simulation modeling of the process was set up in two ways. The first method would appear to be the straightforward natural way to simulate the process. As results demonstrate, it gives incorrect predictions of heat-transfer area requirements.

Two Aspen *HeatX* blocks with counter-current flow are used as shown in Fig. 3. The hexane flowrate is 90 kg/s. In the evaporator, the pressure is 1.25 bar and the *U* is $1.4 \text{ kW m}^{-2} \text{ K}^{-1}$. The hot air enters at 90 °C. In the condenser, the pressure is 0.273 bar and the *U* is 0.85 kW m⁻² K⁻¹. The cooling water enters at 25 °C and leaves at 30 °C. Its flowrate varies from case to case as the design optimization variables are changed. An Aspen *Design spec/vary* function is used to change cooling water flowrate to maintain a 30 °C cooling water exit temperature.

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