DESIGN OF PENTANE VAPORIZERS – A CFD APPROACH

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ABSTRACT
Heat Exchangers (HEs) transfer heat energy from the source to the motive fluid, are a major component of the installation and maintenance costs and have a significant bearing on performance and efficiency of the plant. HEs are usually designed conservatively due to lack of detailed predictive models. Optimised designs can lead to reduced costs and increased plant efficiency.

The project develops an approach for CFD analysis of single-phase and phase-change heat exchangers. CFD models have been validated against experimental data for simple geometries. For multi-tube geometries, the validation is of a qualitative nature because of a lack of experimental data. The final aim of the project is to perform the CFD analysis of a commercial pentane vaporizer (horizontal orientation) (Figure-7). The main objectives are:
a) To understand the impact of liquid level on the heat transfer performance of the Vaporizer
b) To know the probability of droplets being carried into the superheater by the hot vapor flow

At the current stage – a) single-phase CFD models have been validated, b) multi-phase models (which need to be tuned on a case-by-case basis) have been validated for single-tube geometries. Lack of experimental data for pentane boiling has necessitated selection of a surrogate fluid to validate model set-up which has been done on the basis of thermophysical properties and dimensionless numbers that characterize the boiling phenomenon, viz. bubble Reynolds number, Morton number, Eotvos number, Weber number, Boiling number and Jakob number.

1. INTRODUCTION

1.1 Challenges for a vaporizer in duty

The vaporizer is a critical component in a power generation system. It is where the motive/working fluid undergoes change of phase to power the prime rotor (expander) and generate electrical or shaft power. Figure 1 shows a schematic of an organic Rankine cycle power plant of the type of interest for the present work. It has been estimated that more than half of the heat exchangers employed in process industries involve two-phase flow on the shell-side [16], and yet two-phase flow patterns in cross-flow have received much less attention than in-pipe two-phase flow patterns. There have been a number of experimental studies on various single and multi-tube geometries [15, 16, 17, 21, 31, 34, 37, 49] with main focus on areas such as void-fraction prediction correlations and frictional pressure drop prediction correlations. The void fraction and pressure drop measurements obtained by these investigators produced bundle average or pitch average values that were used in the formulation of various correlations.

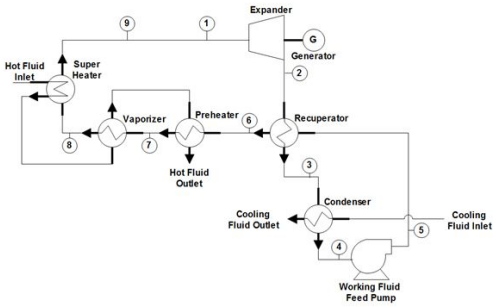


Figure 1 - General schematic representation of an Organic Rankine Cycle power plant

These correlations were formulated without any reference to the flow phenomena that occurred in the passages between the tubes. For example, shell-side two-phase frictional multiplier correlations are extensively used. They are based on the assumed similarity with pipe frictional pressure drops. However, shell-side pressure drop is mechanistically different; as the pipe flow pressure drops are due to wall friction, whereas shell-side pressure drops are due to flow separation and re-attachment phenomena [9].

1.2 Construction Requirements

The vaporizer has to be thermally efficient, easy to clean, robust and cost efficient. Cleaning is particularly important where the hot source fluid carries dissolved minerals, as is usually the case in geothermal applications. Better design requires a deeper understanding of the influence of mechanical (geometrical) parameters (tube surface characteristics, tube pitch, tube diameters, and tube layout) and operational parameters (temperatures and pressures of fluids, scaling of tubes) on the heat transfer during phase change process. High heat transfer performance and cost & ease of cleaning are conflicting goals.

1.3 Thermal Design

The thermal design of the vaporizers is complex due to the physics behind the boiling process. In boiling, mass, momentum and energy transfer (single- and two- phase) involving a solid wall, liquid and vapor are all tightly coupled [28]. There are a number of factors that affect the boiling process and the mechanism and extent of their influence is not fully understood due to a lack of well-established mechanistic models and the lack of computational resources to simulate the phase change, boiling process on large geometries (e.g. Shell –and-Tube Vaporizers, Plate Heat Exchangers (PHEs)).

1.4 Bubble Dynamics

The dynamics of bubble generation and departure are still being investigated and are not fully understood. There are three main models/hypotheses for heat transfer bubble generation and departure process:

- The "Transient Conduction Model" (Han & Griffith(1965), Mikic & Rohsenow(1969))

- "Microlayer Heat Transfer Model" (Snyder & Edwards(1956), Moore & Mesler(1961), Hendricks & Sharp(1964), Cooper & Lloyd(1969))
- "Contact-line Heat Transfer Model" (Stephan & Hammer(1994))

In recent experimental investigations the mechanisms of heat transfer during bubbling events under pool boiling conditions have been studied on micro-scales, the different mechanisms have been properly delineated and their relative contributions measured and presented. The dominant mechanisms have been found to be transient conduction and micro-convection. For example, [28] states that the dominant heat transfer mechanisms are transient conduction and micro-convection (bubble agitation) while the microlayer evaporation and contact line heat transfer have a less than 25% contribution. Myers et.al. (2005) have put forward findings similar to [41], also presented results limiting the contribution of microlayer evaporation to maximum of 28.8% (in agreement with [38]), and negligible contribution by contact line heat transfer mechanism; and the contribution of micro-convection was observed to increase as the wall temperature increased, while transient conduction is more dominant at lower surface temperatures.

The main mechanisms are therefore transient conduction and micro-convection with their relative dominance a function of surface temperature; transient conduction dominating at low surface temperatures and micro-convection dominating at high surface temperatures. Another significant finding is that transient conduction starts well before the bubble departure, which is in complete contrast to the usual definition of transient conduction in boiling literature.

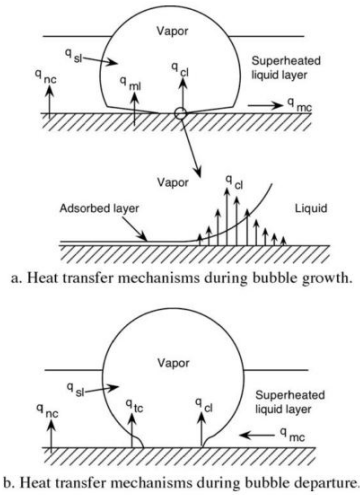


Figure 2 - Various heat transfer mechanisms during bubble formation and departure, [28]

1.5 Void Fraction

The prediction of void fraction inside vaporizers is of utmost importance if we want accurate prediction of local heat transfer coefficient, since heat transfer mechanisms, and hence the correlations required for their prediction, change as the flow pattern changes with increasing void fraction value [32]. There are three main types of flow models that can be used for the prediction of void fraction values, and their use depends on the particular application. These are the: a) Homogeneous flow model, b) In-tube flow model, c) Separated flow model.

Several investigators have proposed void fraction correlations, e.g. Schrage et.al. (1988), Dowlati et.al. (1990) and Feenstra et.al. (2000); while Ishihara et.al. (1980), Xu et.al. (1998) and Simovic et.al. (2007) have proposed methods for frictional pressure drop [9, 16, 34, 37, 49]. Also, most of the studies done to develop two-phase void fraction prediction models used adiabatic two-phase flows [29], which is quite different from actual operating conditions, where the vapor is generated on the tubes and thermo-hydraulic parameters keep changing in both vertical and horizontal directions inside a tube bundle.

1.6 Empirical Modeling vs. Mechanistic Modeling

Originally, the process of heat exchanger design has been based on empirical correlations and formulas developed by a number of researchers based on experimental data and observations and using coefficients/exponents for data fitting. It is an effective technique for designing equipment with similarities in geometry and operating conditions during the experiments, but it fails in being a universal method and also does not represent the extent and manner of influence of different factors that affect the final thermal performance of heat exchangers.

1.7 Basic Sizing Calculations

Heat exchangers are usually over-designed due to following factors:

- Allowance made for degraded performance due to fouling or mineral scaling
- Current design methods not being highly accurate thus necessitating a significant over-design, 15-20%, to guarantee performance. As a consequence of many uncertainties in the predictive models for heat transfer in flooded-type evaporators, safety margins taken for the thermal design of heat exchangers are quite large, and result in an overly conservative design of vaporizers [1, 30, 37].

Challenges towards development of more efficient & accurately sized heat exchangers include:

- Experimental investigation on industrial sized full-scale heat exchangers is prohibitively expensive
- Highly accurate predictive models of mechanistic type have also been developed (in addition to numerous empirical correlations available), but are limited by their requirement of the knowledge of local thermo-hydraulic conditions which are generally not available [37].
- The design of a heat exchanger needs to keep in mind both the heat transfer performance and the accompanying pressure drop, and it is seen mostly that the steps required to increase heat transfer performance lead to higher pressure drop.

1.8 Consideration and Selection of Different Models to be used for Thermal Design

The choice of the model to be used for thermal design of HEs depends on the duty the heat exchanger has to perform, viz. single-phase heating (preheater, superheater) or phase-change (vaporizer) or it can be a combination of these duties. These models are of empirical or semi-empirical nature. The currently available models can be divided into two broad categories: a) reduced-pressure based correlations which predict the boiling heat transfer from macroscopic heat perspective, and b) thermophysical-properties based correlations which are developed on the basis of the microscopic heat transfer mechanisms [8]. Bell-Delaware

[44] is a very detailed method and is very accurate in estimating the shell-side heat transfer coefficient and pressure drop for commonly used shell-and-tube heat exchanger (STHE) geometries. Another option is the Kern method [27], which gives conservative results and is only suitable for preliminary sizing. A promising model for predicting heat transfer in a vaporizer is presented by [30, 29]. Unlike previous approaches, model by [29, 30] recognizes different flow regimes and calculate different Reynolds and Prandtl numbers according the void fraction value, and uses different approaches to calculate the local heat transfer coefficient.

The models for designing can be divided into categories based on the type of user as well, a) For consumers who want to know if their HE is performing optimally and efficiently by comparing the actual outlet conditions to the ones predicted by theoretical models. One such approach was presented by [14]. b) For designers who have to design a heat exchanger from the start for a prescribed duty.

A different approach has been put forward by [19], which takes into account the microphysics of bubble dynamics to calculate the total boiling heat flux. The contributions (towards heat flux, W/m^2) taken are – latent heat by bubbles (q_{LH}), transient conduction (q_{CON}), heat transferred by natural convection (q_{NC}), represented as:

$$q_{tot} = \left(q_{LH}.\tau_g + q_{CON}.\tau_w\right)f + q_{NC}$$

Here, the τ_g is the bubble growth period, and τ_w is the bubble waiting period, and ' f ' denotes the bubble departure frequency.

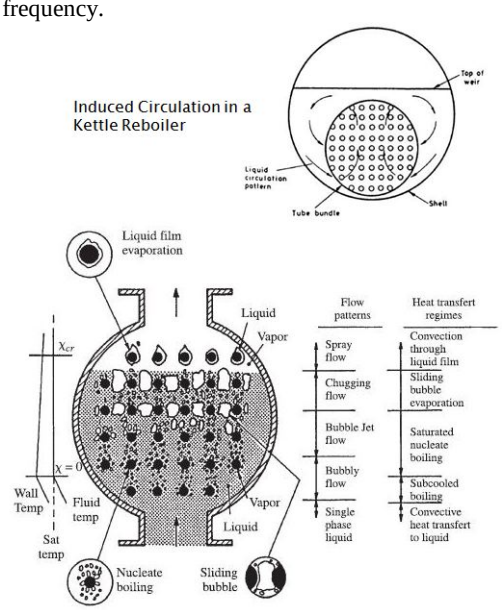


Figure 3 - Representation of flow patterns (a) and flow regimes (b) in a multi-tube vaporizer [26, 45]

2. CFD ANALYSIS

CFD simulations offer the possibility of improving upon existing designs and testing new designs for any industrial equipment due to the fact that it is economically non-viable to manufacture full scale prototypes of all candidate designs. CFD simulations form a filter mechanism at a fraction of a cost of actual manufacture and testing to narrow down on a few final designs that can be then manufactured and tested.

A CFD approach to design of heat exchangers can be classified into two categories: a) single-phase (e.g. preheaters, superheaters), and b) phase-change (e.g. vaporizers, condensers). Multi-phase demands significantly more complexity and computational resource. There is a large literature on single phase heat transfer [2, 11, 18, 20, 22, 23, 24, 25, 33, 35, 36, 39, 40, 42, 46, 47, 48, 50] but fewer papers on phase change, with majority of them focussing on simple geometries such as annuli in an attempt to improve (existing) or validate (new) models that can then be included in newer versions of CFD software. Review of the literature found no articles dealing with phase change in large vaporizer-like geometries that compared CFD analysis against experimental data such as mean bubble diameter or other parameters that define bubble dynamics. The CFD model, especially models defining bubble generation, need to be tuned with the help of experimental data. Table 1 is a brief review of the various sub-models that need to be selected and tuned for phase-change CFD. Table 2 shows the availability of experimental data for water and refrigerants at different operating pressure conditions. No literature was found regarding pentane-boiling at pressures characteristic of multi-megawatt power plants. This lack of experimental data is resolved and explained later in the paper.

MODEL DEVELOPMENT

CFD Solver: ANSYS CFX 15.0
• **Method**: Thermal Phase Change Method (Based on Kurul & Podowski's Wall Heat Flux Partitioning Method)
• Variable Thermophysical Properties
• Sub-models:
  • Bubble departure diameter—Tolubinski-Kostanchuk, Unal, Fritz, Cole Rohsenow, Kocamustafaogullari
  • Wall nucleation site density—Lemmert-Chawla
  • Total interfacial force: Drag force + Lift force + Wall Lubrication force + Turbulent Dispersion Force
  • Drag Force—Schiller Naumann, Ishii Zuber, Grace, Drag Coefficient
  • Lift force—Lift coefficient, Tomiyama, Saffman Mei, Legendre Magnaudet
  • Wall Lubrication force—Antal, Tomiyama, Frank
  • Turbulent Dispersion force—Favre Averaged drag force, Lopez de Bertodano, Simonin
• CFX Expression Language Routines used for:
  • Saturation temperature variation
  • Bulk Bubble Diameter modelling
  • Bubble Departure Diameter modelling
  • Wall roughness modelling

Table 1 - CFD Model Development

CFD Model Validation Data Availability	HIGH PRESSURE	LOW PRESSURE
WATER	HIGH	LOW
REFRIGERANTS	VERY LOW	MEDIUM

Table 2 - Availability of experimental data to validate CFD models

2.1 Single-phase CFD

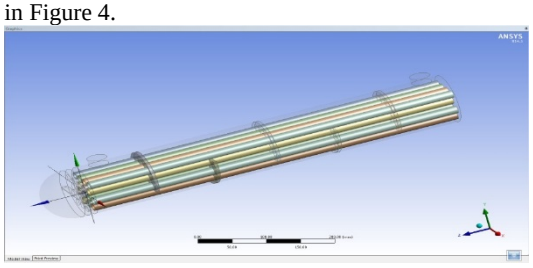
In a power plant, single-phase heat transfer takes place in preheaters and superheaters. There are a number of geometrical factors which affect the performance of these HEs, with the major ones being – baffle height and spacing, tube-to-baffle gap and design of inlet and outlet sections of the shell. Empirical design methods fail to provide effective visualization of the impacts of these geometrical factors. Single-phase CFD simulation has neither large computational requirements nor does it need to be tuned for individual cases. This makes it an extremely desirable and effective tool for design of components that have single-phase heat transfer.

The results for conjugate single-phase heat transfer in a simple TEMA-E type STHE were compared to prediction from the Bell-Delaware method (Table-3). The cases analyzed in the paper have a significant difference to the ones found in the literature due to the fact that conjugate heat transfer is accounted for by simulating both source (hot fluid) and working fluid, rather than using heat flux as the boundary condition. This makes the simulation set-up same as the real world situation and Bell-Delaware method. The theoretical validation (Table-3) proves the validity and feasibility of the single-phase CFD with.

	Method used for prediction	Shell side Outlet Temp. (K)	Tube side Outlet Temp. (K)	Total Heat Duty (kW)
Case-1: SSMFR = 0.1 kg/sec TTMFR = 0.1 kg/sec	MATLAB (Bell-Delaware)	338.41	361.25	16.48
	CFD Simulation (AnsysFLUENT)	339.50	359.88	16.66
		0.3 %	0.3 %	1.1 %
Case-2: SSMFR = 0.2 kg/sec TTMFR = 0.1 kg/sec	MATLAB (Bell-Delaware)	323.86	351.93	20.28
	CFD Simulation (AnsysFLUENT)	323.19	352.96	19.52
		0.2 %	0.29 %	3.7 %
Case-3: SSMFR = 0.3 kg/sec TTMFR = 0.1 kg/sec	MATLAB (Bell-Delaware)	322.33	357.26	27.88
	CFD Simulation (AnsysFLUENT)	320.71	360.09	26.11
		0.5 %	0.79 %	6.3 %

Table 3 - Theoretical Validation of single-phase CFD (SSMFR – Shell Side Mass Flow Rate, TSMFR – Tube Side Mass Flow Rate (per tube))

The simulations were carried out using single-phase heat transfer set-up in ANSYS Fluent (15.0) on geometry shown in Figure 4.



GEOMETRY DETAILS:
Shell Length = 576mm
Number of tubes = 14
Number of baffles = 5

MESH DETAILS:
Unstructured, 0.66m Nodes, 3.28m Elements

Figure 4 - Geometry (with few details) used for theoretical validation. Results shown in Table-3

The plots in in Figure 5 demonstrate the visualization potential unique to CFD simulation and which can be used to understand internal flow structures in various types of HEs e.g. shell-and-plate HE, helical baffled HEs, and simple STHE. CFD simulations can be used to check flow maldistribution issues and effects of baffle cut and baffle spacing [11].

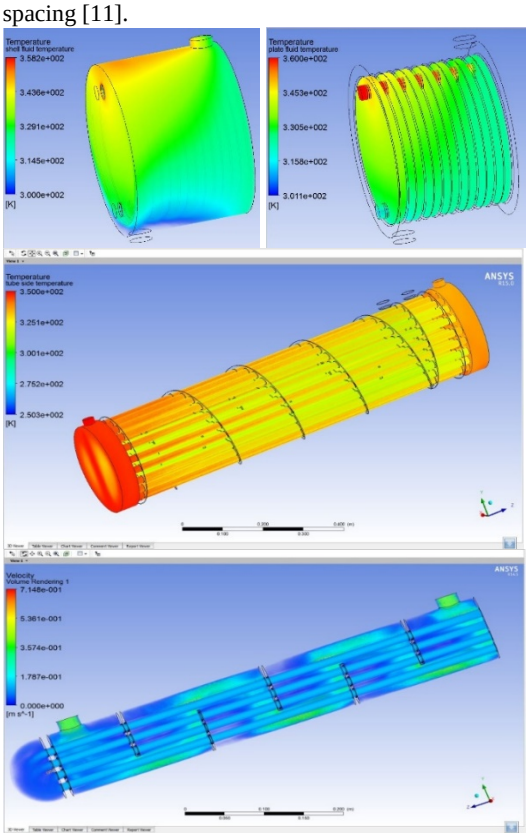


Figure 5 - (a) Temperature Volume Rendering (Shell-side fluid temperature), (b) Temperature Volume Rendering (Plate-side fluid temperature), c) Tube-side temperature volume rendering, conjugate heat transfer, (d) Velocity volume rendering, Baffled STHE

2.2 Phase-change CFD

CFD analysis of phase-change heat exchangers (e.g. vaporizers) requires more sophisticated approaches. The modelling of phase change process is an inherently complex process, and the sheer complexity of geometry and large sizes of industrial vaporizers make the simulation process demanding in computational resources. It is necessitated because the use the alternative simpler methods may predict deficiencies in design but are unable to pin point the location and possible factors of weaknesses.

The CFD analysis of a vaporizer is more complex than CFD analysis of a single-phase heat exchanger (preheater/superheater) due the interaction at interface between two phases which gives rise to various types of flow fields or local interfacial structures. A model with two-fluid (liquid & gas), four-field (continuous & dispersed for both

liquid & gas) approach can allow for the definition of eight types of local interfacial structures as shown in Figure 6.

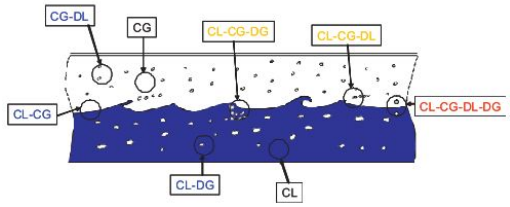


Figure 6 - Illustration of different types of Local Interfacial Structure, [6]

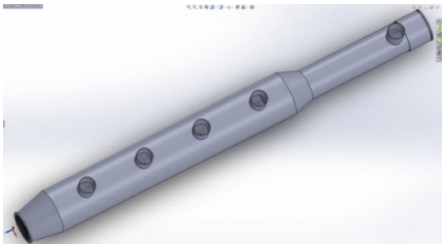


Figure 7 - CAD model of the pentane vaporizer

Figure 7 shows the full scale 3-D model of the pentane-vaporizer, the study of which is the aim of this project. It is not possible to do a CFD analysis of the complete vaporizer with the currently available computer systems because of the computational (especially memory) and time limitations. Considering the internal baffle structure of the vaporizer under the four vapor outlets, a vertical slice was chosen for CFD analysis. This was possible because the internal baffle structure consists of periodically repeating units (Figure 8).

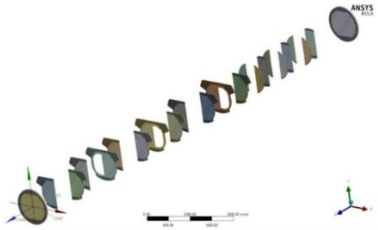


Figure 8 - Internal baffle structure

The selection of a vertical slice (Figure 9) does impose one limitation on the CFD analysis, viz. the effect of inlet and outlet geometry must be accounted for by careful selection of boundary conditions.

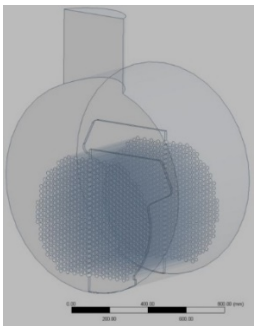


Figure 9 - Vertical slice chosen for CFD analysis

It is necessary to validate CFD model set-ups to have confidence in the results and make predictions based on these results. There is limited experimental data available for multi-tube configurations with phase-change and the literature found refers only to pressure & temperature readings and general flow patterns while no data is recorded pertaining bubble generation and void fraction which are required for setting up and tuning a CFD model to simulate the experiment. No literature was found regarding experiments of boiling of pentane over multi-tube configurations providing measured parameters such as void fraction and mean bubble diameters. Validation in such cases would therefore be limited to a qualitative nature. This necessitates that the physics and parameters used in the model for multi-tube configurations be quantitatively validated against experimental data. This exercise also delineates the main parameters that need to be tuned to match the CFD results to experimental data.

There is however available a vast literature on single tube boiling. At first, the set-up was validated (quantitatively & qualitatively) against three such experiments:

- Upward subcooled boiling of R113 at Arizona State University, analysed by [7].
- Low pressure upward subcooled boiling flow of water, experiments by [43] and analysed by [13, 12].
- Boiling of water in a high-pressure pipe-flow configuration with heat applied at outer boundary of the tube. Experiments by [4, 5], analysed by [10].

The model set-up needs to be tuned for each individual validation study against experimental data but the general approach remains uniform. The tuning is usually required for following parameters:

- Bulk bubble diameter
- Bubble departure diameter
- Thermophysical properties should be variable (either using CFX library or user-defined functions in CFX Expression Language (CEL))

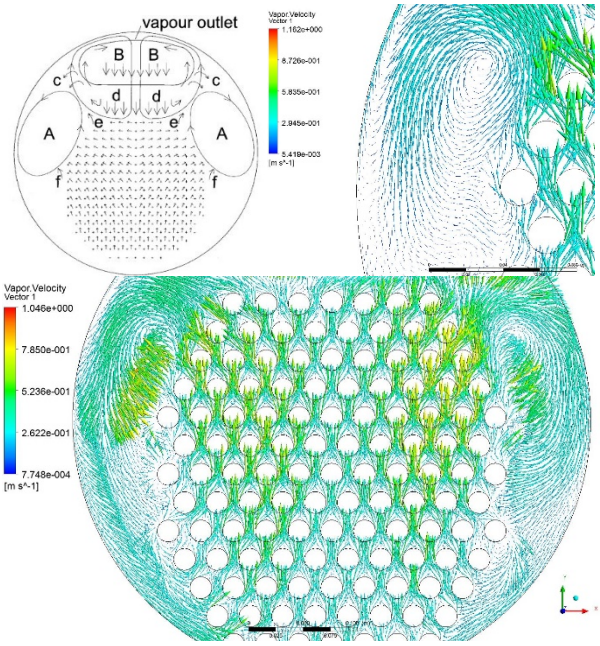


Figure 10 - Experimentally observed (a) [3] and CFD predicted (b, c) vapor flow pattern

The next step was to apply the learnings from single tube boiling models (i.e. how to select and tune models defining

bubble generation) to multi-tube configurations and perform validations against experiments.

In Figure 10, it is observed that the vapor flow pattern predicted by the CFD analysis qualitatively matches the experimentally observed flow pattern. The vapor patterns at the top of the geometry used in CFD analysis are not similar to the experimentally observed patterns as the experimental observation are on a HE with outlet at one side of the length of the shell whereas the CFD analysis is done on a thin section with inlet and outlet in a straight line w.r.t. each other. Figure 11 shows that the variations in heat transfer coefficient along the periphery of a tube as predicted by experimental observation are replicated by CFD simulations. The CFD results shown below are with different operating conditions (w.r.t. pressure) than the experiment and 30^o tube layout instead of in-line (as in experiment).

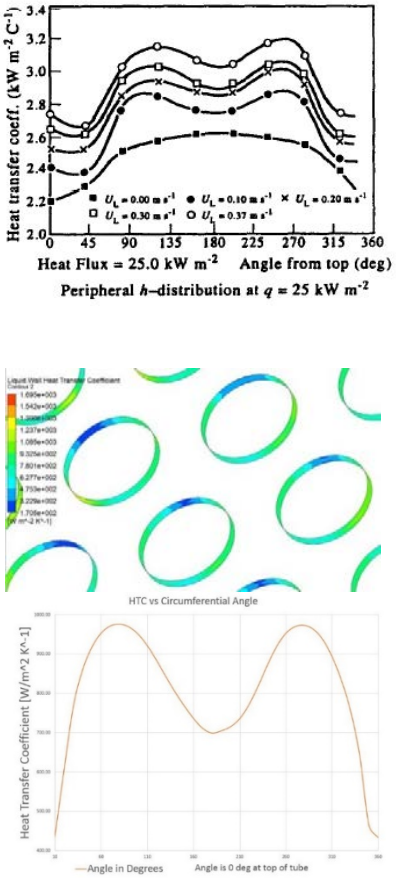


Figure 11 - Experimentally observed (a) [3] and CFD predicted heat transfer coefficient (HTC) (b, c) along the circumference of a tube

While using CFD analysis for a case with little or no experimental data available to validate and tune the model set-up, it becomes both essential and complicated to ascertain factors that can lend confidence into the model set-up. The process of bubble generation needs to be correctly modeled in the CFD model set-up to match simulation results to the experimental data. Bubble generation depends on the thermophysical properties of the liquid undergoing vaporization. The effect of these properties on boiling and bubble generation can be studied by analyzing following dimensionless numbers: Bubble Reynolds number, Morton number, Eotvos number, Weber number, Boiling number and Jakob number. If the pattern of variation thermophysical properties w.r.t. pressure is similar between two fluids then it stands to reason that they exhibit similar changes in bubble dynamics with pressure changes. A comparison (Figure 12) of the variation of thermophysical properties (*enthalpy, density, entropy, specific heat, thermal conductivity, saturation temperature, surface tension & viscosity*) vs. pressure between pentane, R113 and water reveals similar patterns of change among pentane and R113. This led to selection of R113 as a fluid, CFD model set-ups for which can be used as a basis for setting up models for pentane. Another advantage of choosing R113 is the vast literature available on R113-boiling experiments.

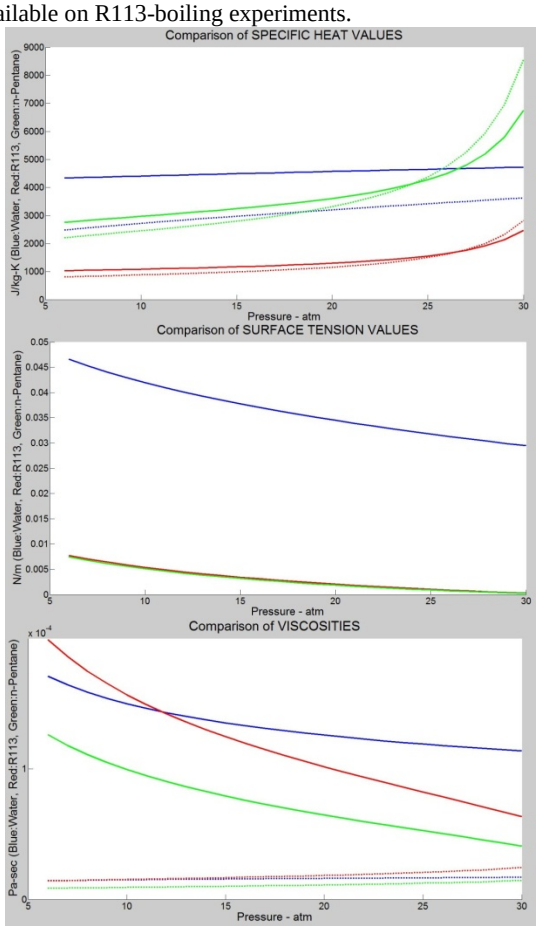


Figure 12 - Comparison of enthalpy (a), surface tension (b) & viscosity (c); Note: Solid lines - Liquid, Dotted lines – Vapor (Red – R113, Green – n-Pentane & Blue – Water)

A comparison (Table-4) of the dimensionless numbers used to characterize boiling and bubble generation between pentane and R113 is done with assumed values of bubble mean diameter & relative velocities between phases. This comparison reveals that the pressure values at which dimensionless numbers have same values for the two fluids match closely for all cases except Eotvos number, pressure values for which are still within an order of magnitude of each other.

The comparisons of a) variation in thermophysical properties, and b) dimensionless numbers used to characterize the boiling process demonstrate the suitability of using R113 model set-ups as basis of models for pentane vaporization.

		Value	Pressure (atm)	
Dimensionless numbers affecting Bubble Dynamics				
Bubble Reynolds Number	n-Pentane	2000	1.97e+01	[For mean bubble diameter = 2
	R113	2000	1.58e+01	

Morton Number	n-Pentane	4e-11	1.97e+01	mm]
	R113	4e-11	1.38e+01	
Eotvos Number	n-Pentane	7	1.79e+01	
	R113	7	6.91e+00	
Dimensionless numbers affecting Boiling				
Weber Number	n-Pentane	240	1.97e+01	[For gas phase velocity = 2 m/s, Relative phasic velocity = 2 m/s]
	R113	240	1.48e+01	
Boiling Number	n-Pentane	1e-02	1.97e+01	
	R113	1e-02	1.96e+01	
Jakob Number	n-Pentane	2.5	1.97e+01	
	R113	2.5	1.58e+01	

Table 4 - Comparison of dimensionless numbers, used to characterize boiling phenomenon, between R113 and pentane

2.3 Future Work

To achieve the two main objectives of the project an approach has been developed and is briefly described here. The impact of liquid level on the heat transfer performance of a vaporizer will be done with the help of a number of parametric studies. To study the process and possibility of droplet carryover the vapor velocity field will be obtained from CFD post-processing and a MATLAB code will be used to determine what sizes of the droplets can be carried out of the vaporizer. There is no experimental data available about the sizes of the droplets that are generated in this particular vaporizer configuration but minimum and maximum sizes of the droplets can be determined. The minimum size is determined by vaporization as droplets below a particular diameter will be vaporized by the hot vapor stream that is carrying them. The maximum size of the droplets will be determined by drag forces and gravity as droplets bigger than a particular size will fall back into the vaporizer.

3. CONCLUSION

The CFD analysis has a great potential to invigorate the design and development process of novel heat exchangers. At the same time it has the power to improve our insight into the workings of currently installed heat exchangers. A comprehensive knowledge of the correlations that exist between various parameters of a heat exchangers gives us the power to optimize the operating conditions and extract maximum performance.

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