

UNIVERSIDADE ESTADUAL DE CAMPINAS

Faculdade de Engenharia Mecânica

HUGO MARMORI DE MORAIS

Modelagem do aquecimento de combustível a altas pressões

Fuel heating modeling at very high pressure

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Modelagem do aquecimento de combustível a altas pressões

Dissertação de Mestrado apresentada à Faculdade de Engenharia Mecânica da Universidade Estadual de Campinas como parte dos requisitos exigidos para a obtenção do título de Mestre em Engenharia Mecânica, na Área de Térmica e Fluidos.

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Orientador: Prof. Dr. Rogério Gonçalves dos Santos

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UNIVERSIDADE ESTADUAL DE CAMPINAS FACULDADE DE ENGENHARIA MECÂNICA

DISSERTAÇÃO DE MESTRADO

Modelagem do aquecimento de combustível a altas pressões

Fuel heating modeling at very high pressure

Autor: Hugo Marmori de Morais

Orientador: Prof. Dr. Rogério Gonçalves dos Santos

A Banca Examinadora composta pelos membros abaixo aprovou esta Dissertação de Mestrado:

Prof. Dr. Rogério Gonçalves dos Santos, Presidente UNICAMP/FEM

Prof. Dr. Fabio Toshio Kanizawa UNICAMP/FEM

Profa. Dra. Debora Carneiro Moreira PPGEMec/UFSCar

A Ata de Defesa com as respectivas assinaturas dos membros encontra-se no SIGA/Sistema de Fluxo de Dissertação/Tese e na Secretaria do Programa da Unidade.

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RESUMO

A partida a frio é um problema bem conhecido na indústria automotiva. A injeção direta é uma das soluções para este problema, pois ela leva a uma melhor atomização do combustível na câmara de combustão. Porém, o aquecimento do combustível melhora as características do spray e também facilita a evaporação do combustível criando uma mistura mais homogênea. No processo de aquecimento uma alta potência é aplicado através de uma pequena superfície, o que pode resultar em ebulição do combustível em pressões inferiores à pressão crítica, e em convecção natural com forte variação de propriedades a pressões superiores à crítica. O objetivo deste trabalho é modelar a transferência de calor por ebulição e convecção natural em altas pressões, buscando aplicá-la em motores de injeção direta. Para a ebulição nucleada, avaliamos 5 correlações de coeficiente de transferência de calor para componentes puros, cinco correlações para misturas e três equações de estados. As métricas de avaliação foram o desvio global, desvio global absoluto e o intervalo de erro de 30%. Duas correlações para componentes puros se sobressairam, Gorenflo e Kenning (2010) e Ribatski e Jabardo (2003), enquanto que nas misturas as correlações tiveram resultados similares. Já as equações de estado não apresentaram grande influência. Conhecida a melhor combinação, foi feita a previsão do coeficiente de transferência de calor a altas pressões para etanol, gasolina e misturas. Para a gasolina, as duas correlações de componentes puros não apresentaram grandes divergência, já para misturas e etanol, quanto maior a quantidade do álcool, maior a distancia entre as correlações. Além disso, próximo ao ponto crítico ocorre um rápido crescimento do coeficiente de transferência de calor. Para a convecção natural supercrítica, foi utilizado uma abordagem diferente. Foram realizadas simulações transientes de convecção natural para o etanol supercrítico com diferentes fluxos de calor em uma geometria 2D similar a um aquecedor de combustível. Em seguida, foi avaliado o comportamento do fluido durante a simulação e comparou-se os coeficientes de transferência de calor da simulação com correlações de convecção natural para cilindros concêntricos. Para que o fluido supercrítico passe a afetar a convecção natural devido a sua rápida variação de propriedades perto do ponto pseudocrítico, é necessário certo nível de fluxo de calor em pressões determinadas. É recomendado utilizar propriedades na média integral quando a o fluido atinge temperaturas acima da temperatura pseudocrítica. Existem indícios de um regime turbulento no topo da geometria do aquecedor.

Palavras-chave: Etanol, Gasolina, ebulição em piscina, convecção natural, fluido supercrítico

ABSTRACT

Cold start is a well-known problem in the automotive industry. Direct injection is one of the possible solutions, because higher injection pressures improves fuel atomization. However, heating the fuel improves the mixture formation, making it more homogeneous. In the heating process, a high heat level is applied across a small surface area, which can result in fuel boiling at pressures below the critical pressure, and in natural convection with strong property variation at pressures above the critical pressure. The objective of this present study is to model heat transfer by boiling and natural convection at high pressures, seeking to apply it in direct injection engines. For nucleate boiling, we evaluated five heat transfer coefficient correlations for pure components, five correlations for mixtures, and 3 equations of states. The metrics for analysis were global deviation, absolute global deviation, and 30% error interval. Two correlations for pure components stood out, Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003), while in the mixtures the correlations had similar results. On the other hand, the equations of state did not show great influence. Once the best combination was known, the heat transfer coefficient was predicted at high pressures for ethanol, gasoline, and blends. For gasoline, the 2 pure component correlations did not show great divergence. For blends and ethanol, the greater the amount of alcohol, the greater the distance between the correlations. Close to the critical point, a rapid increase in the heat transfer coefficient occurs. For supercritical natural convection, a different approach was used. Transient supercritical natural convection simulations were performed for ethanol with different heat fluxes in a 2D geometry similar to a fuel heater. Then, the behavior of the fluid during the simulation was evaluated and the heat transfer coefficient from the CFD were compared with correlations. For the supercritical fluid to affect natural convection due to its rapid change in properties near the pseudocritical point, a certain degree of heat flux at certain pressure levels is required. Average temperature properties are suitable when the fluid reaches temperatures above the pseudocritical temperature. There are indications of a turbulent regime at the top of the heater geometry.

Keywords: ethanol, gasoline, pool boiling, natural convection, supercritical fluid

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LIST OF ABBREVIATIONS AND ACRONYMS

- BIP Binary interaction parameters Cubic Equation of State CEOS **Computational Fluid Dynamics** CFD Cubic Plus Association CPA DI Direct injection Equation of state EOS GDI Gasoline direct injection Hydrocarbon HC Heat transfer coefficient HTC Port Fuel Injection PFI Peng-Robinson PR SRK Soave-Redlich-Kwong
- VLE Vapor-liquid equilibrium

LIST OF SYMBOLS

Roman Letter

a	Attractive fluid-dependent constant
b	Parameter b for cubic equation of state
B_0	Scaling factor - [-]
C	Number of components - $[-]$
C_s	Li <i>et al.</i> (2014)'s correlation constant - $[-]$
c_p	Specific Heat - $[W/kgK]$
d	Break-off diameter - $[m]$
e	Laplace Constant - [-]
f	Fugacity - [Pa]
F	Influence factor for Gorenflo and Kenning (2010)'s correlation - $[-]$
f_w	Heater material constant for Ribatski and Jabardo (2003)'s correlation - $[-]$
g	Gravity acceleration - $[m/s^2]$
g	Gravity vector - $[m/s^2]$
Gr	Grashof number - [-]
h	Heat transfer coefficient - $[W/m^2K]$
Н	Helmholtz free energy - $[J]$
i	Specific enthalpy - $[J/kg]$
j	A property
K	Deterioration factor - [-]
k	Thermal conductivity - $[W/mK]$

k_{ij}	Binary interaction parameter
L	Reference length - $[m]$
M	Molecular Weight - $[g/mol]$
m	Acentric influence factor
N_i	Number of bonding sites on component i - $[-]$
Nu	Nusselt number - [-]
Oh	Ohnesorge number - [-]
Р	Pressure - [bar]
Pr	Prandtl number - [-]
q	Heat flux - $[W/m^2]$
q	Heat flux vector - $[W/m^2]$
r	Cylinder radius - $[m]$
R	Universal gas constant - $[J/K]$
R_a	Mean surface roughness - $[\mu m]$
R_p	Peak surface roughness - $[\mu m]$
Re	Reynolds number - $[-]$
S	Degrees of freedom of a system - $[-]$
T	Temperature - $[^{\circ}C]$
t	Time - [-]
u	Reference velocity - $[m/s]$
u	Velocity vector - $[m/s]$
v	Specific volume - $[m^3/kg]$
w	Heater material influence - $[-]$

X_i	Non-bonded sites fraction
x_i	Molar composition of component i on liquid phase - $[mol/mol]$
y_i	Molar composition of component i on gas phase - $[mol/mol]$
z	Molar composition on overall system - $[mol/mol]$

Greek Letter

u	Thermal diffusivity - $[m^2/s]$
eta	Contact angle - [°]
ρ	Density - $[kg/m^3]$
μ	Dynamic viscosity - [Pa s]
ν	Cinematic viscosity - $[m^2/s]$
σ	Surface tension - $[N/m]$
η	Pressure influence factor on heat flux for Ribatski and Jabardo (2003)'s correlation - $[-]$
ζ	Pressure influence on heat flux for Gorenflo and Kenning (2010)'s correlation - $[-]$
ΔT	Temperature difference - $[^{\circ}C]$
	F
λ	Volume expansion coefficient - $[1/K]$
λ	Volume expansion coefficient - $[1/K]$ Stress tensor - $[Pa]$
λ au Π	Volume expansion coefficient - $[1/K]$ Stress tensor - $[Pa]$ Number of phases - $[-]$
	Volume expansion coefficient - $[1/K]$ Stress tensor - $[Pa]$ Number of phases - $[-]$ Accentric factor - $[-]$
	Volume expansion coefficient - $[1/K]$ Stress tensor - $[Pa]$ Number of phases - $[-]$ Accentric factor - $[-]$ Temperature function of a
$\begin{array}{c} \Delta \\ \lambda \\ \tau \\ \Pi \\ \omega \\ \kappa \\ \phi \end{array}$	Volume expansion coefficient - $[1/K]$ Stress tensor - $[Pa]$ Number of phases - $[-]$ Accentric factor - $[-]$ Temperature function of a Fugacity coefficient - $[-]$

χ	Chemical potential - $[J/mol]$

Subscript

avg	Average
bp	Boiling range
С	Critical property
C	Cooper (1984)'s correlation
CHF	Critical heat flux
exp	Experimental
ext	External
f	Fluid
fg	Vaporization
F, 1994	Fujita and Tsutsui (1994)'s correlation
F, 1997	Fujita and Tsutsui (1997)'s correlation
G	Gorenflo and Kenning (2010)'s correlation
g	Vapor
Ι	Inoue et al. (1998)'s correlation
i	Component i
id	Ideal
int	Internal
l	Liquid
Li	Li et al. (2014)'s correlation
Р	Pressure influence
pc	Average critical property

PR	Peng-Robison
pred	Prediction
q	Heat flux influence
r	Reduced property
ref	Reference value
res	Residual
RJ	Ribatski and Jabardo (2003)'s correlation
S	Saturation
SA	Stephan and Abdelsalam (1980)'s correlation
SRK	Soave-Redlich-Kwong
Т	Thome (1983)'s correlation
TS	Thome and Shakir (1987)'s correlation
w	wall

Superscript

L	Liquid phase
V	Vapor phase
$\alpha \text{ or } \beta$	Phase
0	Reference state

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1 INTRODUCTION

The world has been looking for ways to reduce the amount of pollutant emitted, which can be achieved by a less harsh production, a more environmental friendly fuel, a better engine performance. Researchers studied several alternative energy sources, consequently, different technologies became reality: electric vehicles, hydrogen is an option for internal combustion engines (ICE) and fuel cells, and several applications use biofuel (Abrar *et al.*, 2023).

1.1 Ethanol

The search for an alternative fuel to reduce the consumption of fossil fuel date back to the oil crisis in the last century. THe search for a cheaper fuel when the world faced an increase in petroleum prices boosted the research on ethanol. In 1975, Brazil created the program PROALCOOL, which was focused on developing the use of ethanol as a fuel (Stolf; Oliveira, 2020), following the first oil crisis. The investments made in the program allowed Brazil to develop ethanol fueled engine and reduced Brazilian dependency on fossil fuels. Then the flex fuel engine were developed, which can use gasoline, ethanol, or a blend of those in any proportion (Marques *et al.*, 2017). This contributed to transform ethanol in an alternative to gasoline in vehicles.

Ethanol is a renewable energy source because it is harvested from sugarcane, corn or biomass of organic compounds residues. The possibility of the production from residues, referred as second generation ethanol, is an advantage for using ethanol as it would not compete with the food production (Correa *et al.*, 2022), although in Brazil the production comes directly from agriculture. Also, Brazil has an electric grid where a big part of the energy comes from renewable sources, decreasing the CO2 emitted to produce ethanol, and making it more environmental friendly than in other countries (Pacheco; Silva, 2019).

Also, ethanol has a higher octane number, decreasing knock, and a lower emission of carbon monoxide (CO) and hydrocarbon (HC). It is easy to handle and transport (Bae; Kim, 2017), and can be added to gasoline, which decreases the emission of pollutants in comparison to pure gasoline (Nakata *et al.*, 2006; Lou *et al.*, 2023).



Figure 1.1 – Gasoline auxiliary system schematic drawing. Source: (Kabasin et al., 2009)

1.2 Cold start

However, ethanol has a bad cold start performance in ICE. At low temperatures, ethanol has difficulty reaching the flash point and has bad atomization (Bae; Kim, 2017), process of formation of small droplets, which makes it difficult and troubling for the engine to start. Without assistance, an ethanol-fueled engine cannot start at temperatures below $13^{\circ}C$ (Sales; Sodré, 2012). To solve this problem, three solutions (Kabasin *et al.*, 2009; Oliveira *et al.*, 2016) can be used a gasoline auxiliary system, a fuel heating system or the direct injection. The first consist of a separated system with a tank of gasoline that would provide gasoline to start the engine. The second is an equipment that heats the ethanol approximating it to the flash point condition. An additional system with gasoline is not desirable, because of the amount of additional required components and the necessity to keep a level of gasoline in the car's extra reservoir. Figure 1.1 shows a schematic drawing of a gasoline auxiliary system (Kabasin *et al.*, 2009).

Also, cold start represents part of the engine operation and impacts pollutant emissions. The cold start emissions are an expressive part of CO, PN, and NOx emitted during the engine operation (Du *et al.*, 2020). At low temperatures, the fuel atomization deteriorates (Nigra, 2016; Fajgenbaum, 2013), and so does the combustion. The evaporation is decreased, which contributes to the formation of liquid fuel films and consequently to the production of soot (Stevens; Steeper, 2001; Witze; Green, 1997). Contrasting with the cold phase of the engine, at the fully warmed-up condition the performance of the ICE is better (He *et al.*, 2022).

1.3 Direct Injection

Direct injection (DI) is a method of producing air-fuel mixture, in which fuel is injected directly into the combustion chamber. The fuel flows to the cylinder during the compression cycle of the four-stroke internal combustion engine. The DI method has already been applied to Diesel engines, but in recent times, it has been incorporated into Otto engines (Brunetti, 2018) to substitute the port fuel injection (PFI). In PFI, the fuel is injected inside of the intake manifold with the air, they mix before they are injected into the combustion chamber, and the air-fuel mixture enters the cylinder in the admission phase of the four strokes. The PFI mixes better the fuel with air, while DI has a much lower time to create a homogeneous mixture between air and fuel, creating locally rich mixtures of fuel (He *et al.*, 2022). However, the direct injection achieves better volumetric efficiency, higher knock resistance, and better fuel economy due to more accurate control of the fuel injected (Sens; Rieß, 2018).

The mixture formation of air-fuel DI engines depends on the nozzle and the properties of the fuel injected. The properties will determine the breakup regime of the fuel mostly based on the combination of two dimensionless numbers, Reynolds and Ohnesorge numbers,

$$Re = \frac{uL\rho}{\mu} \tag{1.1}$$

and

$$Oh = \frac{\mu}{\sqrt{\sigma L\rho}},\tag{1.2}$$

respectively. In the Reynolds number, ρ is the density of the fluid, u is the characteristic velocity of the flow, L is the characteristic flow length, μ is the dynamic viscosity, and in the Ohnesorge number, σ is the surface tension. Figure 1.2 shows the spray regime according to both Reynolds and Ohnesorge numbers (Sens; Rieß, 2018). The aimed regime is the atomization one, where the fuel forms very small droplets that improve the heat transfer and the mass transfer (Brunetti, 2018). It can be achieved by increasing fuel temperature, because the higher temperature will decrease dynamic viscosity and surface tension.

1.4 Fuel heating

Based on the previous discussion, it is interesting to preheat the ethanol, before it is injected into the combustion chamber, aiming to favor the atomization process and to reduce the pollutant emission. One of its applications is to solve ethanol's cold start problem (Kabasin



(a) Spray break up regimes according to the Reynolds and Ohnesorge numbers. Source: (Sens; Rieß, 2018)



(b) Spray break up regimes visualization

Figure 1.2 – Spray break regimes. Source: (Sens; Rieß, 2018)

et al., 2009), but it can be further extended to direct injection ICE. Direct injection suffers from wall wetting, fuel impingement, and low-quality mixture formation. One of the ways to overcome this issue is through an increase in fuel temperature (Oliveira *et al.*, 2016).

Figures 1.3a and 1.3b show two possible locations for the fuel heater, which may change according to the manufacturer, and the fuel rail and fuel injector (Netto *et al.*, 2022). The heater is always in contact with the fuel. The heating process is triggered by an external action from the driver, like opening the car's door or deactivating the alarm system, from there on the heater starts to transfer energy to the fluid on high heat fluxes. Figure 1.4 shows how the system works, providing energy to the fuel, and then keeping the fuel temperature until the end of the engine cold phase. The amount of energy per unit of area is so high that nucleate pool boiling may occur. When the engine starts, fuel flows from the fuel rail through the fuel injector into the air intake if it is a PFI system, or into the combustion chamber if it is a DI system. The fuel heater usually stops after the engine is heated.

Sens and Rieß (2018) showed that increasing the temperature decreases the droplet

fuel size in a more effective way than increasing the pressure. Fedor *et al.* (2016) found that the emission of hydrocarbon in gasoline direct injection (GDI) decreases with fuel heating. Because the heated fuel evaporates easier, it will improve mixture quality (Koga *et al.*, 2001; Miganakallu *et al.*, 2023) and reduce the amount of liquid formed inside of the heating chamber and the wall wetting.

If fuel is heated at high pressures, higher than the critical pressure, it can achieve the supercritical state. Fuel-injected at this condition reduces pollutant emission and increases efficiency, because supercritical fuel creates a more homogeneous air-fuel mixture due to low viscosity, high mass diffusion, and low surface tension (Song *et al.*, 2020).

Despite being a promising solution, modeling fuel heating at high pressures lacks in research. It is necessary more experimental data, correlations were not tested on high-pressure conditions, and the studies focus on lower pressure levels and alternative surfaces. Recent studies proposed a surrogate for gasoline to model pool boiling, but it was not tested with high pressure (Netto *et al.*, 2022).

There is no study of the capabilities of the current models in extending them to higher pressures. Dahariya and Betz (2019) compared different correlations with experimental data, however, the highest pressure tested is 5 bar. New studies present correlations based on neural networks (Calati *et al.*, 2021; Sajjad *et al.*, 2021), but its reproduction has a randomness level. Other studies are interested in dielectric fluids for electronic cooling applications (Tran *et al.*, 2020).

1.5 Objective of the present work

This study concerns the modeling of fuel heating processes at very high pressures, near the critical point, providing how to predict the heat transfer coefficient (HTC) between the fuel and the heater, for further applications on fuel heaters. The HTC prediction helps to design fuel heaters by providing a magnitude order of HTC and consequently the temperatures involved in heat transfer. The secondary objectives are to analyze the accuracy of several combinations of Equations of State, mixture nucleate boiling correlation, and pure component nucleate boiling correlation, and to evaluate the transient fuel heating at a pressure higher than the critical one.

This study is structured in five chapters. The second chapter is a review of the theory necessary for the analysis: nucleate pool boiling, natural convection, supercritical fluids, equation of state (EOS) and phase equilibrium. On the third chapter, the methodology and



(b) Fuel heater located on the path to the fuel injector.

Figure 1.3 – Fuel heater schematic drawing



Figure 1.4 – Schematic drawing of the fuel heater operation. Source: Netto et al. (2022)

results modeling the boiling phenomenon at pressures below the critical one is presented. On the forth chapter, it is the part for the natural convection of supercritical fluids to be modeled. The fifth chapter concludes the study.

2 LITERATURE REVIEW

Heat goes from higher temperature regions to lower temperature regions and there are 3 ways: conduction, convection and radiation. A solid that presents a point of higher temperature will transfer its energy from molecule to molecule, diffusing heat, this is known as conduction. In conduction, there is no movement of the parts involved. However, a heated fluid that is in movement can carry its energy to another location, or even remove heat from a surface flowing over it. This is known as convection, when the heat is transferred with movement. Another way of transferring heat is through electromagnetic waves. All bodies emit thermal radiation, but the ones that receives more energy than it emits, increase its temperature (Bejan; Kraus, 2003).

Convection can occur through phase change, when the heat flows from one location to another, and change of physical state happens. If this process of adding heat transform liquid into vapor, it is known as boiling (Rohsenow *et al.*, 1998). It is divided in two types: pool boiling and flow boiling. The first is the phenomenon in an initially stationary fluid where the movement is caused only by natural convection or phase change, and in the second, the fluid flow because of a external force. The boiling phenomenon is used at several industrial processes - electronic processors, nuclear reactors, rocket motors cooling (Tong; Tang, 2018) - because it has a high heat transfer coefficient (HTC).

2.1 Boiling curve

There are several regimes of pool boiling, and they depend on the level of wall superheating or the heat flux. Figure 2.1 shows the pool boiling curve, it represents how the heat flux or the wall superheating behaves when the other is controlled, and also separates the boiling regimes. The blue lines and arrows show the path when the heat flux is controlled, and the black lines and arrows show the deviation from the established path when the temperature is controlled. Heat flux and temperature difference are related by Newton's cooling law:

$$q = h\Delta T. \tag{2.1}$$

where q is the heat flux, h is the HTC and ΔT is the temperature difference between the bulk liquid temperature and the wall temperature. In the lower heat flux range, there is only natural

convection with no formation of bubbles, as the heat flux increases and achieves the onset nucleate boiling (ONB) heat flux, the formation of bubbles starts (Tong; Tang, 2018). From this point until the critical heat flux, it is known as nucleate pool boiling, where bubbles are formed and sustained after a certain heat flux or temperature difference, the formation of bubbles increases the HTC, decreasing the wall temperature. After the critical heat flux, the wall temperature increases very fast so it keeps the heat flux level when the heat is controlled. However, if the wall temperature is controlled, the level of heat flux decreases until it reaches the Leidenfrost point, the location of the minimum heat flux. This region is known as transition boiling because of concomitant existence of nucleate and film boiling regimes. In the film boiling, a thin vapor film forms between the wall and the liquid part of the fluid (Çengel; Ghajar, 2020), the heat is transferred from the solid surface to the liquid portion through radiation and conduction across the vapor film.



Figure 2.1 – Pool boiling curve

2.2 Nucleate Pool Boiling

Pool boiling is one of the processes that boiling can occur. In this case, there is flow movement generated by natural convection and bubble formation. The vapor is generated in the region of contact between the heated surface and the liquid (Çengel; Ghajar, 2020).

A vapor nucleus can be generated at the heated surface or can already exist before the beginning of pool boiling if the vapor is trapped there, or there is non-condensable gas. The boiling phenomenon will start when the liquid temperature achieves a higher temperature than the saturated one (Bejan; Kraus, 2003). A boundary layer is formed, transitioning from the wall temperature to liquid saturation temperature. As the heat is added, more liquid vaporizes, the a bubble grows, separates and rises from the vapor nucleus disrupting the boundary layer. The surrounding liquid fills the gap left by the bubble and the process restarts by reforming the boundary layer.

To increase its size, the bubble receives heat from different sources:

- the boundary layer, which is a layer that temperature decreases from wall temperature to bulk liquid temperature
- the microlayer, which is a thin film of liquid trapped between the growing bubble and the heated surface (Gao *et al.*, 2013);
- the three-phase contact line, which is a region where the liquid, the vapor, and the solid heated surface are in contact;
- the micro convection, due to the perturbations in the liquid caused by the growing bubble (Kim, 2009).

A part of the heat that converts the liquid to vapor comes from the boundary layer (Demiray; Kim, 2004), on the other hand, the microlayer depletes when the bubble is growing, decreasing the temperature locally (Theofanous *et al.*, 2002), indicating a point of high HTC.

For mixtures, the boiling phenomenon changes due to the existence of a less volatile component. The most volatile will evaporate easily, but it will make the less volatile to concentrate closer to the heater surface, increasing the temperature near the wall (Inoue, 1991; Fujita; Tsutsui, 1994).

The pool boiling process is a very complex phenomenon with no analytical solution. Experimental correlations are usually used to predict heat transfer coefficients that aggregate information from the fluid, the heater, and how they interact between them. Through the years, several correlations have been proposed for pure components and mixtures. They can depend on other empirical correlations for nucleate site density, and bubble diameter, while others require knowledge of the contact angle. All of these values might make the use of correlations hard (Guichet *et al.*, 2019).

Pure component nucleate pool boiling correlation cannot predict well HTC for mixture, even though mixture properties are used for it (Fujita; Tsutsui, 1994). In mixtures, the HTC deteriorates due to the accumulation of less volatile components in liquid phase (Oliveira, 2017), a local phenomenon that pure component correlations are not fitted for. So it is not possible to use an ideal HTC

$$h_{id} = \frac{1}{\sum_{i=1}^{n} z_i / h_i},$$
(2.2)

where h_{id} is the ideal HTC, z_i is the molar composition of component *i* on the mixture, and h_i is the HTC of component *i* on the same state of the mixture. From h_{id} , it is possible to calculate the ideal ΔT_{id}

$$\Delta T_{id} = \frac{q}{h_{id}}.\tag{2.3}$$

However, a deterioration factor K is incorporated so it changes the HTC to a lower value (Netto, 2020)

$$h_{mix} = \frac{h_{id}}{1+K}.$$
(2.4)

The value K will depends on the correlation used, it is a function of the thermophysical and transport properties, the vapor-liquid equilibrium curve - mainly the bubble and dew point (Sathyabhama; Babu, 2011).

Correlations can represent well the experimental data that they are fitted, but may achieve poorer results when compared to other data (Fujita; Tsutsui, 1994). They can also have an empirical constant for every mixture. Some correlations present the mass transfer coefficient, which can be treated as an experimental parameter from each mixture. These parameters can make the correlations difficult to use because they require the correct value of these constants for every mixture (Fujita; Tsutsui, 1997).

The correlations that are presented in the following subsections are used in the rest of the study. They are easy to use and provide reference values for unknown properties, like Stephan and Abdelsalam (1980)'s correlation, which provides a value for the contact angle.

2.2.1 Pure component correlations

• Stephan and Abdelsalam (1980)

Their correlation uses an approach based on transport and thermodynamic properties. There are correlations for the following types of fluids: water, refrigerant, hydrocarbon,
and cryogenic fluids

$$Nu = 2.46 \times 10^7 \left(\frac{qd}{k_l T_s}\right)^{0.673} \left(\frac{i_{fg}d^2}{\alpha_l^2}\right)^{-1.58} \left(\frac{c_{p,l} T_s d^2}{\alpha_l^2}\right)^{1.26} \left(\frac{\rho_l - \rho_g}{\rho_l}\right)^{5.22}, \quad (2.5)$$
$$10^{-4} \le P_r \le 0.886, \ \beta = 45^{\circ}$$

$$Nu = 0.0546 \left[\left(\frac{\rho_g}{\rho_l} \right)^{0.5} \frac{qd}{k_l T_s} \right]^{0.67} \left(\frac{\rho_l - \rho_g}{\rho_l} \right)^{-4.33} \left(\frac{i_{fg} d^2}{\alpha_l^2} \right)^{0.248},$$

$$5.7 \times 10^{-3} \le P_r \le 0.9, \ \beta = 35^{\circ}$$
(2.6)

$$Nu = 4.82 \left(\frac{qd}{k_l T_s}\right)^{0.624} \left(\frac{\rho c_p k}{\rho_l c_{p,l} k_l}\right)^{0.117} \left(\frac{\rho_g}{\rho_l}\right)^{0.257} \left(\frac{c_{p,l} T_s d^2}{\alpha_l^2}\right)^{0.374} \left(\frac{i_{fg} d^2}{\alpha_l^2}\right)^{0.329},$$

$$4 \times 10^{-3} \le P_r \le 0.97, \ \beta = 1^{\circ}$$
(2.7)

$$Nu = 207 \left(\frac{qd}{k_l T_s}\right)^{0.745} \left(\frac{\rho_g}{\rho_l}\right)^{0.581} \left(\frac{\nu_l}{\alpha_l}\right)^{0.533},$$

$$3 \times 10^{-3} \le P_r \le 0.78, \ \beta = 35^{\circ}$$
 (2.8)

Nu is the Nusselt number, it is a ratio between convected and conducted energy

$$Nu = \frac{hL}{k},\tag{2.9}$$

where L is the reference length, k the thermal conductivity, and h the HTC. For Stephan and Abdelsalam (1980)'s correlation, HTC will be denominated h_{SA} . There is an equation for all substances

$$Nu = 0.23 \left(\frac{qd}{k_l T_s}\right)^{0.674} \left(\frac{\rho_g}{\rho_l}\right)^{0.297} \left(\frac{i_{fg} d^2}{\alpha_l^2}\right)^{0.371} \left(\frac{\rho_l - \rho_g}{\rho_l}\right)^{-1.73} \left(\frac{\alpha_l^2 \rho_l}{\sigma d}\right)^{0.35}, \quad (2.10)$$
$$10^{-4} \le P_r \le 0.97,$$

where σ is the surface tension.

The parameter d is the break-off diameter,

$$d = 0.0146\beta e, (2.11)$$

 k_l is the thermal conductivity, T_s is the saturation temperature, α_l is the liquid thermal diffusivity, ρ_l is the liquid density, $c_{p,l}$ is the liquid specific heat at constant pressure, i_{fg}

is the vaporization enthalpy, ρ_g is the vapor density, ν_l is the liquid cinematic viscosity, β is the contact angle, e is

$$e = \left[\frac{2\sigma}{g(\rho_l - \rho_g)}\right]^{1/2},\tag{2.12}$$

which is the Laplace constant, and g is the gravity acceleration.

• Cooper (1984)

Cooper (1984) proposed a simplification of the existing correlations

$$h_C = 55q^{0.67} P_r^{(0.12 - 0.2\log_{10}R_p)} (-\log_{10}P_r)^{-0.55} M^{-0.5},$$
(2.13)

where P_r is the reduced pressure, R_p is the peak roughness and M is the molecular weight

• Ribatski and Jabardo (2003)

The correlation uses heat flux, reduced properties, surface roughness, surface material, and molecular parameter, to achieve the following correlation

$$h_{RJ} = q^{\eta} f_w P_r^{0.45} [-log(P_r)]^{-0.8} R_a^{0.2} M^{-0.5}, \qquad (2.14)$$

$$\eta = 0.9 - 0.3 P_r^{0.2} \tag{2.15}$$

where R_a is the mean surface roughness, and f_w is a constant that depends on the heater material. f_w can be 100 for copper, 110 for brass, 85 for stainless steel, (Ribatski; Jabardo, 2003), and 56 for platinum, which was later proposed by Oliveira (2017)

• Gorenflo and Kenning (2010)

Their correlation corrects the value of the heat transfer coefficients from standard values. The HTC is calculated as

$$\frac{h_G}{h_{ref}} = F_q(q)F_P(P_r)F_w \tag{2.16}$$

where h_{ref} is the value of the HTC at the reference condition of $20 kW/m^2$ and reduced pressure of 0.1, F_q is the heat flux influence factor, F_p is the pressure influence factor and F_w is the heater material and surface influence factor. All of these factors are calculated as:

$$F_q = \left(\frac{q}{q_{ref}}\right)^{\zeta(P_r)}; \qquad (2.17)$$

$$\zeta(P_r) = 0.95 - 0.3P_r; \tag{2.18}$$

$$F_p = 0.7P_r^{0.2} + 4P_r + \frac{1.4P_r}{1 - P_r};$$
(2.19)

$$F_w = \left[\frac{R_a}{R_{a,ref}}\right]^{2/15} \left[\frac{(k\rho c_p)_w}{(k\rho c_p)_{Cu}}\right]^{0.25};$$
(2.20)

where Ra_0 is the reference roughness average, k is the thermal conductivity, ρ is the density and c_p the specific heat at constant pressure, w subscript represent the wall, and Cu represents copper. The reference HTC can be calculated by

$$h_{ref} = 3580 \left[\frac{(dP/dT)_{sat}}{10^6 \sigma} \right]_{P_r=0.1}^{0.6}$$
(2.21)

where σ is the surface tension and $(dP/dT)_{sat}$ the slope of the saturation curve.

• Li et al. (2014)

Another correlation that requires the fluid thermodynamic and transport properties is Li *et al.* (2014)'s correlation. Their correlation is associated with Rohsenow's correlation, but it has corrections for the interaction between the heater and fluid

$$h_{Li} = \frac{1}{0.013C_s^{-0.33}(c_{p,l}\mu_l/k_l)} \frac{qc_{p,l}}{i_{fg}} \left(\frac{\mu_l i_{fg}}{q\sqrt{\frac{\sigma}{g(\rho_l - \rho_g)}}}\right)^{0.33},$$
(2.22)

$$C_s = \sqrt{1 - \cos(\beta)} \left[1 + \frac{5.45}{(R_a - 3.5)^2 + 2.61} \right] w^{-0.04},$$
(2.23)

where w is the heater material influence

2.2.2 Mixture correlations

• Thome (1983)

He presents a correlation that removes the non-linear terms due to physical properties variation. The correlation is also easily extended for multi-component mixtures because of its simplicity. The deterioration factor is

$$K_T = \frac{\Delta T_{bp}}{\Delta T_{id}},\tag{2.24}$$

where ΔT_{bp} is the temperature difference between dew and bubble point. It is calculated through Vapor Liquid Equilibrium problem.

The deterioration factor is used on equation (2.4). However, there is a lack of information about the influence of heat flux, which can be detrimental in lower heat fluxes.

• Thome and Shakir (1987)

They incorporated new factors to Thome (1983)'s correlation. The new equation accounts for the influence of the rising local bubble point temperature and was fitted using experimental data from aqueous mixtures. The new equation with the exponential correction is

$$K_{TS} = \frac{\Delta T_{bp}}{\Delta T_{id}} \left[1 - exp\left(\frac{-B_0 q}{\rho_l i_{fg} \beta_l}\right) \right]$$
(2.25)

where B_0 is the scaling factor, and β_l the liquid side mass transfer coefficient, determined as 0.0003 m/s (Sathyabhama; Babu, 2011)

• Fujita and Tsutsui (1994)

A new correlation was fitted using experimental data of several kinds of mixtures: aqueous, non-aqueous, azeotrope, non-azeotrope. Fujita and Tsutsui (1994) modified Thome (1983)'s correlation to implement the influence of the heat flux

$$K_{F,1994} = \left[1 - 0.8exp(10^{-5}q)\right] \frac{\Delta T_{bp}}{\Delta T_{id}}$$
(2.26)

• Fujita and Tsutsui (1997)

Using the same data as before (Fujita; Tsutsui, 1994), a new correlation was proposed. It was derived based on the Kutateladze (1951)'s CHF equation that uses the mixture properties to calculate the CHF like it was a pseudo pure component. The equation is given as follows

$$K_{F,1997} = \frac{\Delta T_{bp}}{\Delta T_{id}} \left\{ 1 - exp \left[\frac{-60q}{\rho_g i_{fg}} \left(\frac{\rho_g^2}{\sigma g(\rho_l - \rho_g)} \right)^{1/4} \right] \right\}.$$
 (2.27)

• Inoue et al. (1998)

This correlation was proposed based on experiments with binary mixtures of refrigerants. The equation incorporates the influence of boiling point rising locally due to the local concentration. An equation was proposed by Inoue (1991), but it did not satisfied the unity condition presented in Inoue *et al.* (1998), so a new deterioration factor was presented

$$K_{I} = \left[1 - 0.75 exp(0.75 \times 10^{-5}q)\right] \frac{\Delta T_{bp}}{\Delta T_{id}}$$
(2.28)

2.3 Critical Heat Flux

The boiling crisis is the fast increase in wall superheating when the critical heat flux (CHF) is achieved (Theofanous *et al.*, 2002), because of the poor wall rewetting. Different authors present different mechanisms to explain CHF. Zuber introduced the hydrodynamic instability, which the CHF would occur due to hydrodynamic instabilities that would prevent the liquid from reaching the wall to wet it (Liang; Mudawar, 2018). As a consequence, Zuber proposed the following equation

$$q_{CHF} = 0.131 \rho_g i_{fg} \left[\sigma g \frac{(\rho_l - \rho_g)}{\rho_g^2} \right]^{1/4}$$
(2.29)

The equation (2.29) estimates accurately the CHF (Yagov, 2014), but it is dependence on a critical velocity was not accurate when compared to experiments (Katto; Otokuni, 1994), where higher vapor velocities did not cause a flow change. Another mechanism is the macrolayer drying out. This layer consists of liquid under a big vapor bubble that is supplied by vapor steam. The burnout would occur when the macrolayer is depleted. A third proposed mechanism is through a irreversible dry spot - a dry point formed in the place where once there was a bubble (Liang; Mudawar, 2018).

2.4 Natural Convection

Natural convection is the heat transfer through the movement of fluid caused by density difference in the fluid. In the case of a mechanical force imposed on, we can have forced convection, when the movement caused by a density gradient can be neglected, or mixed convection, when both of the flow mechanism act and are important (Çengel; Ghajar, 2020). The choice of which convection should be modeled is usually made by looking at the Reynolds, equation (1.1), and Grashof dimensionless number,

$$Gr = \frac{g\lambda(T_w - T)L^3}{\nu^2},$$
(2.30)

where λ is the volume expansion coefficient, T_w is the wall temperature, and T is the fluid temperature far from the wall. If $Gr/Re^2 >> 1$, the natural convection predominates; if $Gr/Re^2 \sim 1$, both kind of convection are important for the flow; and if $Gr/Re^2 << 1$, the forced convection predominates.

Another dimensionless number is constantly used with natural convection, the Rayleigh number

$$Ra = GrPr = \frac{g\lambda(T_w - T)L^3}{\nu\alpha}.$$
(2.31)

This number is a product between the Grashoff and Prandtl number

$$Pr = \frac{\nu}{\alpha} \tag{2.32}$$

The Reynolds number is a ratio between convective force and diffusive force. On the other hand, the Grashof number is the Reynolds number squared, but the point is that the velocity in the Grashof number is induced by the temperature difference and consequently the density gradient (Nellis; Klein, 2008). The Prandtl number is a ratio between , momentum and thermal diffusivities.

Despite being driven by density gradient, the most common model for natural convection is the Boussinesq's (Armengol *et al.*, 2017). This model neglects the density variation but alters the gravity force on the Navier-Stokes equation by introducing the thermal expansion coefficient and the temperature gradient. However, the Boussinesq model needs a series of conditions to be valid: small temperature differences, constant thermophysical properties, small pressure variations, negligible viscous heat dissipation (Mayeli; Sheard, 2021). If these conditions are not satisfied and thermophysical properties are variable, the following system of partial differential equations needs to be solved (Li *et al.*, 2022):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0; \qquad (2.33)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla P + \rho \mathbf{g} + \nabla \cdot \tau; \qquad (2.34)$$

$$\frac{\partial(\rho i)}{\partial t} + \nabla \cdot (\rho \mathbf{u}i) = \nabla \cdot \mathbf{q} - \nabla(\rho \mathbf{u}) + \nabla \cdot (\tau \cdot \mathbf{u}), \qquad (2.35)$$

where **u** is the velocity vector, **g** the gravity vector, τ is the stress tensor, *i* is the specific enthalpy, and **q** is the heat flux vector.

Just like the nucleate pool boiling, natural convection has a lot of correlations for different geometries, Rayleigh and Prandlt numbers, and fluid conditions. For horizontal cylinders with Rayleigh number less than 10^{12} (Çengel; Ghajar, 2020)

$$Nu = \left\{ 0.6 + \frac{0.387 Ra^{1/6}}{[1 + (0.559/Pr)^{9/16}]^{8/27}} \right\}^2.$$
 (2.36)

Armengol *et al.* (2017) found that the Nusselt number for variable properties is bigger than for constant ones.

2.4.1 Concentric cylinder

The concentric cylinder is a geometry composed of two cylinders one inside the other, in 2D, it is known as an annulus. It is a geometry common for fuel heaters. In this geometry, the heated wall is usually located in the inner cylinder and the outer is the cold one. This geometry causes a plume formation right over the top of the heater and usually keeps the higher velocities only on the upper part (Farouk; Güçeri, 1982). Kuehn and Goldstein (1978) conducted experiments of natural convection in concentric cylinder. They present a value for the beginning of turbulence at $Ra = 1.6 \times 10^7$ and fully turbulent at $Ra = 2 \times 10^7$. However, this unsteady behavior stayed only on the upper part of the cylinder. The following correlation can be used to calculate the HTC for the inner cylinder (Kuehn; Goldstein, 1976):

$$Nu = \frac{2}{\ln\left[1 + \frac{2}{\left[(0.518Ra^{1/4}\left[1 + \left(\frac{0.559}{Pr}\right)^{3/5}\right]^{-5/12}\right)^{15} + \left(0.1Ra^{1/3}\right)^{15}\right]^{1/15}}\right]}$$
(2.37)

On Gorenflo and Kenning (2010)'s heat atlas there is another correlation for concentric cylinder

$$Nu = 0.2Ra^{0.25} \left(\frac{r_{int}}{r_{ext}}\right)^{0.5},$$
(2.38)

where r_{int} is the radius of the inner cylinder and r_{ext} the external one.

2.5 Supercritical Fluid

A supercritical fluid is a fluid in a pressure and temperature higher than the critical point. It is known by high properties variation and the lack of interface between liquid and vapor, so it is not possible to differentiate each phase (Pioro, 2020). The strong variation of properties near the critical point is correlated to the balance between the intermolecular potential and the high-velocity collisions (Elliott *et al.*, 2012).

However, we can divide it based on its behavior depending on the region of pressure and temperature. At high pressures above the Frenkel line, it has a solid-like behavior. Below it and above the Widom line, it behaves as a liquid, and below this line, it behaves as a gas. Both lines can be defined through the fluid properties. The Frenkel line is based on the lack of oscillation of velocity autocorrelation function (Chen; Jiang, 2019). And the Widom line can be divided based on different properties that will result in different paths of the Widom line. On pressure levels close to the critical pressure, if we move across the isobaric changing the temperature, we will eventually see a rapid change of several properties like specific heat at constant pressure, expansion coefficient, compressibility coefficient, and density fluctuation. Each of them will achieve a maximum or a minimum of their values, at this point we name it the pseudocritical point, and the combination of these points will lead to the Widom line (Chen; Jiang, 2019). Figure 2.2 show the different lines separating the supercritical region.



Figure 2.2 – P-T phase diagram with Widom lines according to different properties and Frenkel line separating the supercritical regions of rigid-like, liquid-like and gas-like behavior. Source: (Chen; Jiang, 2019)

As a result of a lack of interface, there is no boiling in a supercritical fluid, so convection is the main heat transfer method. However, if the pressure is close to the critical point and the pseudocritical point is within reach, we can observe a pseudo-boiling (Tamba *et al.*, 1998), because the heated fluid that is on the gas-like region will leave the heated surface in a shape similar to a bubble (Pioro, 2020). This phenomenon usually increases the HTC. Meanwhile, it can also happen a pseudo-film boiling, where the fluid in contact with the wall behaves like a gas (Tamba *et al.*, 1998).

Supercritical fluids also show another mechanism of heat transfer, the piston effect, which is a thermoacoustic effect (Li *et al.*, 2014). According to Masuda *et al.* (2002), the piston effect occur when heated fluid has difficulty transferring heat because of the low diffusivity, but its expansion compresses the rest of the fluid. The adiabatic compression rises the temperature

throughout the whole fluid.

Because of the conditions, in which supercritical fluids exist, it is not possible to use the Boussinesq approximation for natural convection. It is necessary to use the traditional equations with variable properties- equations (2.33), (2.34), (2.35)- making its calculation more complicated.

Supercritical fluids have several applications. They are used in nuclear reactors to cool down the reactors (Pizzarelli, 2018), supercritical carbon dioxide is used in extraction process (Li *et al.*, 2022). They can also be used for thermal energy storage (Luz *et al.*, 2022).

2.6 Equation of State

To find out how many variables we need to know to define a thermodynamic state, the phase rule equates

$$S = C - \Pi + 2 \tag{2.39}$$

where S is the degrees of freedom of a system, C is the number of components, and Π the number of phases. For a fluid with only one component and phase, only 2 properties are required to determine its state and eventually calculate its properties (Klein; Nellis, 2011). It is preferred to get thermodynamic properties directly from experiments of pure components or mixture (Elliott *et al.*, 2012), but this is not a viable option due to the large number of fluids and mixtures. A possible solution is to use an equation of state (EOS), a mathematical relation between thermodynamic properties that describes the fluid or mixture behavior or state.

The most common EOS is the ideal gases equation

$$Pv = RT, (2.40)$$

where P is the absolute pressure, v the specific volume, R the universal gas constant, and T the absolute temperature. This equation has a lot of simplification hypotheses and works well with several gases at low pressures (Klein; Nellis, 2011). However, it can not predict the saturation condition where two phases coexist, and it does not work with liquids. Also, as the pressure increases, it loses accuracy, because the molecules start to interact with each other, which violates one of the ideal gas law hypothesis. Therefore, equation (2.40) do not fit more complex situations. So a more universal EOS is required, one that could work in several situations.

2.6.1 Van der Wall EOS

In this context, Van der Wall proposed his equation in 1873 using the experimental data available at the time, the equation is (Klein; Nellis, 2011)

$$P = \frac{RT}{v - b_{VW}} - \frac{a_{VW}}{v^2}$$
(2.41)

where a_{VW} and b_{VW} are fluid-dependent constants that represent the attractive forces and the volume occupied by the molecule (Valderrama, 2003), respectively. Both constants can be fitted experimentally or by implying the condition

$$\frac{\partial P}{\partial v}\Big|_{T} = 0$$

$$\frac{\partial^{2} P}{\partial v^{2}}\Big|_{T} = 0$$
(2.42)

at the critical point (Klein; Nellis, 2011).

2.6.1.1 Soave-Redlich-Kwong (SRK)

The Soave-Redlich-Kwong is a cubic equation of state described as follows

$$P = \frac{RT}{v - b_{SRK}} - \frac{a_{SRK}\kappa}{v(v + b_{SRK})}$$

$$\kappa = [1 + m_{SRK}(1 - T_r^{0.5})]^2$$

$$m_{SRK} = 0.48 + 1.574\omega - 0.176\omega^2$$
(2.43)

where ω is the acentric factor, which contributes to specifying the vapor pressure curve (Elliott *et al.*, 2012), it is a fluid-dependent variable. a_{SRK} and b_{SRK} are calculated as

$$a_{SRK} = 0.42747 \frac{RT_c^{5/2}}{P_c} \tag{2.44}$$

$$b_{SRK} = 0.08664 \frac{RT_c}{P_c} \tag{2.45}$$

The SRK comes from the modification of the Van der Walls and Redlich-Kwong equation, it incorporates the dependence of the attractive factor over the temperature.

2.6.1.2 Peng-Robinson (PR)

Peng and Robinson proposed a series of modifications by changing the α and the attractive term (Valderrama, 2003), resulting in

$$P = \frac{RT}{v - b_{PR}} - \frac{a_{PR}\kappa}{v(v + b_{PR}) + b_{PR}(v - b_{PR})}$$

$$\kappa = [1 + m_{PR}(1 - T_r^{0.5})]^2$$

$$m_{PR} = 0.37464 - 1.54226\omega - 0.26992\omega^2$$
(2.46)

where

$$a_{PR} = 0.45724 \frac{RT_c^{5/2}}{P_c} \tag{2.47}$$

$$b_{PR} = 0.07780 \frac{RT_c}{P_c} \tag{2.48}$$

This modification allowed better results for vapor-liquid equilibrium (VLE) and liquids.

A series of modifications are constantly proposed to this Cubic EOS, they can improve the EOS performance in specific areas, but that can be detrimental to the overall. So, we decided to use through the study only the original SRK and PR equations. Although they may achieve poorer results for some components and mixtures, they are easier to implement, simpler to extend to mixtures, and have a lot of available data for binary interaction parameters (BIP).

2.6.2 Association Theory (CPA)

The non-idealities presented in hydrocarbon are related to its shape and size, and not to its asymmetric electron distribution (Lira *et al.*, 2022). More complex molecules have polar and hydrogen bond interactions, causing non-idealities in their mixture, which can happen with alcohol, water, and so on.

Oil companies developed the CPA to extend the cubic equation of state (CEOS) so they could capture the effects of associating molecules (Kontogeorgis *et al.*, 2006). Their objective was to combine the capabilities of simple CEOS with the ability to model systems with hydrogen-bonding components. The model combines the SRK equation of state with an additional term from Wertheim's association theory. The CPA is

$$P = \frac{RT}{v - b_{CPA}} - \frac{a_{CPA}\alpha}{v(v + b_{CPA})} - RT \frac{\sum_{i} n_{i} N_{i} (1 - X_{i})}{V - 0.475 b_{CPA}}$$
(2.49)

where N_i is the number of bonding sites on component *i* and X_i is the non-bonded fraction of such sites.

2.6.3 High-accuracy equations

Although the CEOS are easy to use, they lose accuracy in some cases, being preferable to use either empirical correlations or in some cases High-accuracy equations. For example, the reduced Helmholtz equation of state is widely used in software like EES, Multiflash, CoolProp, ANSYS, and so on. This EOS is

$$H(T_r, \rho_r) = H_{ig}(T_r, \rho_r) + H_{res}(T_r, \rho_r)$$
(2.50)

where H is the Helmholtz free energy, ρ_r is the reduced density, and the subscripts *ig* and *res* represent the ideal gas and the residual, respectively (Bell *et al.*, 2014). This kind of EOS is known as a complete equation of state because its thermodynamic properties can be easily calculated analytically through derivatives (Klein; Nellis, 2011).

To represent the residual part of the equation (2.50), several parameters are used and fitted to experimental data (Klein; Nellis, 2011; Schroeder *et al.*, 2014). Depending on the fluid, this information is more restricted, for example, isooctane, or has not been fitted yet.

2.6.4 Mixture rule

EOSs can be extended to a mixture employing mixture rules. Mixture rules describe how the EOS parameters are adapted for a mixture through its composition, pure parameters, and binary interaction parameter (BIP). A simple mixing rule is

$$a_{mix} = \sum_{i} \sum_{j} z_i z_j a_{ij} \tag{2.51}$$

$$b_{mix} = \sum_{i} z_i b_i \tag{2.52}$$

where a_{ij} is

$$a_{ij} = \sqrt{a_i a_j} (1 - k_{ij}),$$
 (2.53)

 k_{ij} is a BIP, z_i is the molar composition.

2.7 Phase Equilibrium

The existence of two phases, according to equation (2.39), implies that only one thermodynamic property is necessary to define the saturation line. But with more components in the mixture, more properties are required, which can be the composition of the system or another thermodynamic property.

Phase diagrams show the existing phases according to the state. On T-x-y diagrams, the pressure is fixed, and temperature and composition are varied. The lower line is the bubble line, it is a frontier between the region of only liquid and the start of the formation of vapor. The upper line is the dew line, which separates the region of liquid and vapor coexistence and the vapor region. If a fluid that is under the bubble line is heated, it will reach this line and vapor will start to form, the composition of the liquid phase is given by the composition where the isothermal line crosses the bubble line, while the vapor phase will be composed of the composition where the isothermal line crosses the dew line. Figure 2.3a shows the T-x-y diagram, where it is the bubble line, dew line the existing phases in each region, and the overall composition of component i, z_i , the liquid composition, x_i , and the vapor composition, y_i .

Both of these lines also appear on the P-x-y diagram, where the temperature is fixed and the pressure and composition are varied. The position of the bubble line and dew line will change on the P-x-y diagram, and so does the state of liquid and vapor. It is important to note that not all mixtures will form a bubble line that covers the whole composition region from 0 to 1. Figure 2.3b shows the P-x-y diagram.

Vapor-liquid equilibrium (VLE) problems are situations where we seek to determine the properties of the vapor-liquid region. To solve this problem, we start with the chemical potential relation

$$\chi_i^{\alpha} = \chi_i^{\beta} \tag{2.54}$$

where χ is the chemical potential, *i* is the component, and α and β represent two phases. We describe the chemical potential using the fugacity, which can be understood as a corrected pressure. Rearranging equation (2.54) we get

$$f_i^{\alpha} = f_i^{\beta}, \tag{2.55}$$

where f is the fugacity. For ideal solutions, this equality can be easily solved using Raoult's law:

$$y_i P = x_i P_i^{sat}, (2.56)$$

where $y_i P$ is the fugacity of component *i* in vapor phase, $x_i P_i^{sat}$ is the fugacity of the component *i* in the liquid phase, x_i is the molar composition of component *i* in liquid phase, and y_i is the molar composition of component *i* in vapor phase. However, this approach is not suited for non-ideal solutions, like isopropanol and water (Elliott *et al.*, 2012), and at higher pressures where the collisions between particles are more frequent.



(a) T-x-y diagram



(b) P-x-y

Figure 2.3 – Schematic of a phase diagram

Another possibility is the $\gamma-\phi$ method. The activity coefficient is

$$\gamma_i = \frac{f_i}{x_i f_i^0} \tag{2.57}$$

where f_i^0 is the fugacity at a standard state. And ϕ is the fugacity coefficient

$$\phi_i = \frac{f_i}{y_i P} \tag{2.58}$$

The equality is given as follows

$$x_i f_i^0 = \phi_i y_i P \tag{2.59}$$

 f_i^0 is the fugacity at a standard state.

The point that separates each VLE method is how the fugacity for each phase will be expressed. The $\gamma - \phi$ method operates with the activity coefficient for the liquid and the fugacity coefficient for the vapor. The liquid fugacity can be calculated utilizing the activity coefficient, γ . The activity models are derived from the excess Gibbs energy, but it is not suited for high pressure. In the $\phi - \phi$ method, the equilibrium is given by

$$x_i \phi_i^L = y_i \phi_i^V, \, i = 1, ..., n \tag{2.60}$$

Using the $\phi - \phi$ method requires an EOSs because the fugacity is evaluated from a standard state and the path from the standard until the desired state must all be covered and valid by an equation. The equation that has that capability is the EOS. It can directly account for the effects of pressure and temperature, and near the critical point, it can capture effects that activity models can't (Lira *et al.*, 2022).

2.7.1 Supercritical Mixture

For supercritical VLE, when one of the components is in the supercritical state, the phase diagram will change, the bubble line and the dew line will bend, and the point they connect is known as a binary critical point (Deiters; Kraska, 2012). For example, figure 2.4 shows the P-x-y diagram for a mixture of ethanol and water at different temperatures, the dew line and the bubble line start to encounter each other when the pressure is higher than the critical for ethanol, 910 psi (62.6 bar) in the figure, creating the critical locus line. This is a line that separates the mixture Vapor Liquid Equilibrium possibility from the supercritical mixture, beyond it, there is only supercritical fluid. Another effect that is visible, is the azeotrope mixture, when dew line and bubble line coincides, common characteristic for ethanol-water mixture (Barr-David; Dodge, 1959). The simplest phase diagram for critical conditions will have a curve that connects the critical points from the pure substances. Some different effects can be found, for example, a mixture in a supercritical state can expand and get inside the phase

envelope condensing the liquid and creating a state with vapor and liquid, then as it expands the liquid will evaporate until it reaches the dew line, where there will be only vapor.



Figure 2.4 – P-x-y ethanol-water diagram at high pressures. Source:Barr-David and Dodge (1959)

2.8 Softwares

Throughout the whole study, several calculations were done for VLE, supercritical fluids, mixtures, and so on. To conduct all the calculations of the thermodynamic properties and transport properties below critical point, we used KBC's software Multiflash. The software has information for several fluids and mixtures, including BIPs, and has equations of state. The software can calculate mixture properties easily and can indicate if the mixture is stable or not. Furthermore, the software has the equation for the components of Netto *et al.* (2022)'s surrogate, which are used to model gasoline for pool boiling phenomenon. The use of commercial

softwares allows faster and broader analysis of the nucleate boiling data. In Multiflash, the model we used for viscosity and thermal conductivity is SuperTRAPP and for surface tension was Linear Gradient Theory.

Other software was tested along the development of the study. CoolProp was the first attempt to calculate the thermodynamic properties. Although it has an interface with Python and uses high accuracy EOS, the software lacked in information for fluids and mainly mixtures.

ANSYS Fluent is used for CFD. Because CoolProp has the same EOS for ethanol present in Fluent, some supercritical calculation were done there for natural convection correlations.

3 HIGH-PRESSURE NUCLEATE POOL BOILING

The fuel nucleate boiling phenomenon is modeled below the critical pressure. Due to the high heat flux values delivered to the fluid in such a small area, the boiling phenomenon occurs. The capability to calculate the HTC helps to determine the temperature difference that the heating system is subjected to.

To start the modeling process, we decided to analyze data gathered in several papers to decide the best combination of correlations and EOS chosen for the fuel heating situation: hydrocarbon and alcohol mixtures, horizontal tube and wire, high pressure, and copper and platinum heater surface. We further compared the correlations with gasoline and blends experimental data (Oliveira, 2017).

Then, we calculated gasoline, ethanol, and gasoline-ethanol blend properties using Multiflash and $\phi - \phi$ method for VLE. Knowing the properties and the correlation best suited for our interests, we predict the HTC behavior for the mixtures cited, gasoline and blends, as the pressure increases.

Figure 3.1 shows the calculation procedure to predict ethanol and blend HTC. The red boxes are choices that have to be made concerning the EOS, or the correlation.

We used the following parameters to measure and analyze the data:

• Overall Absolute Deviation (OAD): the measure of the absolute deviation

$$OAD = \frac{1}{n} \sum_{i=1}^{n} \frac{|h_{pred} - h_{exp}|}{h_{exp}}$$
(3.1)



Figure 3.1 – Methodology steps for predicting HTC of ethanol, gasoline and ethanol-gasoline blends

• Overall Deviation (OD): the measure of how the deviation is distant from the center

$$OD = \frac{1}{n} \sum_{i=1}^{n} \frac{h_{pred} - h_{exp}}{h_{exp}}$$
(3.2)

• γ_{30} : the measure of how many predictions are inside an error interval of 30%

We used three EOS to get the properties, they are SRK, PR, and CPA. PR and SRK are simple cubic equations of state with widespread use, while CPA is a more complicated one because of the association theory term. We opted for this EOS because it works better with associating fluids, like ethanol. All the transport and thermodynamic properties calculations were made using Multiflash software and its Excel interface. We set pressure and molar composition on its functions for bubble and dew point calculations, and the software returns the desired values

3.1 Data analysis

Stephan and Abdelsalam (1980) and Li *et al.* (2014) correlation need contact angles information to calculate the HTC, so the contact angles used are the references provided by Stephan and Abdelsalam (1980) correlation. Li *et al.* (2014) correlation uses a w parameter that depends on the heater surface, we opted to use it as 50, because after 5, w do not affect intensively and the data presented in Li *et al.* (2014) do not show many values below 5. The last assumption made is that for ammonia we used all substances within Stephan and Abdelsalam (1980) correlation, this occur because there is not a class that ammonia could be directly fitted on this correlation.

The data from the papers presented in table 3.1 gather results from a series of fluids, and mixtures, which are binary, ternary, and quaternary. The total data points are 6621. The data can be divided in heater geometry, heater material, type of fluid, and reduced pressure

3.1.1 Pure component

Of the 6621 points, 2760 are from pure components. After removing fluids that were not on Multiflash, we had 2724 data points for the 3 EOS. Figure 3.2 shows the data distribution for fluids, heater material and type, and reduced pressure. The refrigerants dominate the data gathered, with R-134a being the most represented fluid. For heater material, copper has more data points than other materials, while carbon steel has less than 100 data points. For the heater

Reference	Number of points
Inoue <i>et al.</i> (2002)	169
Sun et al. (2007)	364
Sakashita et al. (2010)	111
Shen <i>et al.</i> (1999)	350
Gong <i>et al.</i> (2013)	72
Zhao <i>et al.</i> (2008)	45
Schlindwein et al. (2009)	41
Shi et al. (2010)	306
Sathyabhama and Babu (2011)	94
Fujita and Tsutsui (1994)	628
Dang et al. (2018)	106
Fujita and Tsutsui (2002)	912
Rao and Balakrishnan (2004)	169
Nahra and Næss (2009)	56
Kotthoff and Gorenflo (2008)	44
Köster <i>et al.</i> (1997)	124
Peyghambarzadeh et al. (2009)	84
Sarafraz <i>et al.</i> (2012)	180
Cioulachtjian and Lallemand (2004)	180
Kadhuma <i>et al.</i> (1997)	44
Zhang <i>et al.</i> (2007b)	126
Inoue and Monde (1994)	292
Gorenflo et al. (1988)	92
Zhang <i>et al.</i> (2007a)	54
Gong et al. (2009)	306
Cardoso and Passos (2013)	33
Cardoso et al. (2011)	35
Jung et al. (2004)	40
Jung et al. (2003)	64
Kiyomura <i>et al.</i> (2017)	15
Ribatski and Jabardo (2003)	286
Jabardo et al. (2009)	714
Gorenflo et al. (2004)	106
Jones <i>et al.</i> (2009)	115
Oliveira et al. (2019)	264
Total	6621

Table 3.1 – Papers used and the number of points

type, the most present heater is the horizontal tube. The reduced pressure distribution shows the lack of information about pool boiling at high reduced pressure, most of the data is located between 0 and 0.3, and there are no data points near $P_{red} = 1$, the highest pressure is 0.804 for propane.

3.1.1.1 Overall

For pure component, Gorenflo and Kenning (2010), Ribatski and Jabardo (2003) and Cooper (1984) correlation are not affected by the EOS chosen. They do not rely on thermodynamic or transport properties, with exception of the pressure.

Table 3.2 has the OAD, OD, and γ_{30} data for the different combinations of EOS and pure component correlations. Ribatski's correlation has the best results in every metric analyzed, although the difference of OAD between Ribatski and Stephan is only 0.003 and for γ_{30} between Gorenflo and Ribatski is only 0.001. Cooper has the highest OAD and γ_{30} value, and a tendency to underestimate.

Besides EOSs affecting the results, they are not the main influence factor. Stephan and Abdelsalam (1980) OAD data only changed 0.02, while OAD can increase 0.069 depending on the correlation used. γ_{30} can vary by 0.042 because of EOS, which is smaller when compared to the impact of correlation, around 0.143. So for further pure component analysis, only the Peng-Robison equation of state were used.

Correlation	СРА			PR			SRK		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_{SA}	0.336	0.0340	0.562	0.342	0.0502	0.537	0.356	0.0964	0.530
h_C	0.402	-0.0927	0.420	0.402	-0.0927	0.420	0.402	-0.0927	0.420
h_{RJ}	0.333	0.0114	0.613	0.333	0.0114	0.613	0.333	0.0114	0.613
h_G	0.365	0.0707	0.612	0.365	0.0707	0.612	0.365	0.0707	0.612
h_{Li}	0.363	0.0134	0.470	0.346	-0.0200	0.502	0.337	-0.0441	0.512

Table 3.2 – Overall results for CPA, PR, and SRK using the pure correlations of section 2.2.1

Figures 3.3 shows the distribution of the experimental HTC associated with its corresponding calculated value using Gorenflo and Kenning (2010) correlation. The black line is the best result that can be achieved, and the red lines are the limits for γ_{30} . The graph allows the visualization of data, but, due to the number of data points, some results are hidden and might mislead our judgment. However, it is clear that result for water is underestimated,



(d) Reduced pressure distribution

Figure 3.2 – Data type distribution according to fluid, heater material and type, and reduced pressure for pure component



(b) Smaller HTC

Figure 3.3 – Comparison between the experimental HTC and calculated HTC using Gorenflo and Kenning (2010) correlation for pure components, the black line is the optimum result and the red line is the 30% error

close to the -30% error line, R-134a is widespread across the domain, but the biggest errors are overestimated.

Figure 3.4 show the behavior of each correlation presented in section 2.2.1. Stephan and Abdelsalam (1980) and Li *et al.* (2014) correlations were able to keep propane results inside the γ_{30} . Besides, they both presented similar HTC behavior for water, mainly on high HTC.



Figure 3.4 – Comparison between the experimental HTC and calculated HTC using pure component nucleate boiling correlations and PR

3.1.1.2 Fluid

The focus of this study is on ethanol and gasoline. So, separating the hydrocarbon and alcohol data, we have 526 data points for hydrocarbon and 238 data points for alcohol. The best correlation was Ribatski and Jabardo (2003) as table 3.3 shows the accuracy metrics for the pure component correlation applied to hydrocarbon and alcohol. The OAD is the smaller, while the γ_{30} is the bigger between the correlations analyzed. For alcohol, there is no other correlation that had similar results, the closest OAD is only 0.283, 0.128 distant.

Li *et al.* (2014) correlation had the worst results for OAD and γ_{30} for hydrocarbon, but it is very close to Cooper (1984) correlation, the second correlation with the worst predictions. For alcohol, there is not a correlation that achieves poor results on both OAD and

Correlation		Hydrocarbon	Alcohol			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_{SA}	0.354	-0.000402	0.437	0.350	0.187	0.592
h_C	0.385	-0.0147	0.359	0.329	0.0104	0.517
h_{RJ}	0.304	0.135	0.719	0.155	0.0744	0.853
h_G	0.329	0.133	0.662	0.315	0.0769	0.513
h_{Li}	0.430	0.0580	0.333	0.283	-0.245	0.605

Table 3.3 – OAD, OD, and γ_{30} results for hydrocarbon and alcohol using pure component correlations and PR

 γ_{30} , Stephan and Abdelsalam (1980) correlation that had the highest OAD, and Gorenflo and Kenning (2010) correlation that had the lowest γ_{30} for alcohol.

3.1.1.3 Pressure

The pressure intervals used are:

- Low reduced pressure interval: [0.0, 0.1];
- Middle reduced pressure interval: [0.1, 0.5];
- High reduced pressure interval: [0.5, 1].

We have chosen these pressure levels so there are data points in every interval that do not represent only one fluid, and keep an expressive number of data points for the intervals. With this division, we have 1608, 969, and 147 points for [0.0, 0.1], [0.1, 0.5] and [0.5, 1], respectively. The data for $P_r \ge 0.5$ is composed of refrigerants - R-32, R-22, R-125, R-152a, R-143a and R-114 - and hydrocarbon - Propane and N-butane.

Table 3.4 shows the accuracy metrics according to reduced pressure intervals. For reduced pressures until 0.1, Ribatski and Jabardo (2003) correlation had the best OAD and γ_{30} , with a tendency to overestimate the HTC. On the other hand, Cooper (1984) correlation had the worst results, managing to achieve only 43.8 % of the predictions inside the γ_{30} .

For reduced pressures between 0.1 and 0.5, Gorenflo and Kenning (2010) HTC kept more predictions inside the 30% error range, while had the worst OAD. Also, equation (2.16), tended to overestimate its predictions. The best overall absolute deviation was achieved by Li *et al.* (2014) correlation.

Gorenflo and Kenning (2010) correlation resulted in better predictions at high pressures, $P_r > 0.5$, while the other correlations had similar poor results. The difference from

Correlation	$0 < P_r < 0.1$			$0.1 \le P_r < 0.5$			$0.5 \le P_r < 1$		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_{SA}	0.317	0.0854	0.709	0.369	0.0628	0.521	0.438	-0.419	0.265
h_C	0.404	-0.00907	0.438	0.383	-0.170	0.436	0.499	-0.499	0.129
h_{RJ}	0.273	0.0704	0.709	0.410	-0.0127	0.523	0.435	-0.475	0.156
h_G	0.327	-0.0286	0.554	0.455	0.265	0.673	0.174	-0.123	0.844
h_{Li}	0.334	0.105	0.550	0.322	-0.133	0.499	0.646	-0.646	0

Table 3.4 – OAD, OD, and γ_{30} results using pure component correlations and PR for reduced pressure intervals: [0, 0.1], [0.1, 0.5], [0.5, 1]

Gorenflo and Kenning (2010) OAD to the others correlations can be high as 0.47. This difference level was not seen in other cases. All of the correlations had a great tendency to underestimate the HTC, but equation (2.16) kept its OD near 0.

3.1.1.4 Heater geometry

The geometry analyzed were the horizontal tube and the wire. They were chosen because this is how fuel heaters are usually shaped, for example, Marelli's fuel heater is a cylinder, and Bosch's fuel heater is similar to a wire. With this geometry division, we have 1385 experimental data for horizontal tubes and 604 points for wire.

For horizontal tube, Ribatski and Jabardo (2003) correlation predicted better values for HTC. This correlation achieved 0.321 for OAD and 0.719 for γ_{30} , the best results in these metrics. However, it overestimates with the highest value for OD between the correlations. Stephan and Abdelsalam (1980) correlation got the lowest γ_{30} and Gorenflo and Kenning (2010) got the biggest OAD for horizontal tube.

The wire geometry got different results. Gorenflo and Kenning (2010) correlation combined the best results for all the metrics. It had the lowest OAD, the highest γ_{30} , while it is the most centered correlation because OD is close to 0.

Table 3.5 – OAD, OD, and γ_{30} results using pure component correlations and PR for horizontal tube and wire heaters

Correlation	He	orizontal tu	be	Wire			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_{SA}	0.363	0.00103	0.434	0.345	0.243	0.551	
h_C	0.370	-0.0951	0.500	0.311	-0.0713	0.505	
h_{RJ}	0.321	0.111	0.719	0.342	-0.250	0.459	
h_G	0.422	0.0937	0.571	0.222	0.0466	0.735	
h_{Li}	0.326	-0.0301	0.546	0.388	0.109	0.474	

3.1.1.5 Heater material

Dividing the data by heater material, and selecting the two materials closer to our application, fuel heater, we have 1400 experimental data points for copper and 604 for platinum. The wire data and the platinum data are the same for pure components, so the analysis made in the previous section for wire geometry can be further extended to platinum. However, the lack of diversity forbids to evaluate the difference between platinum and wire influence over the experimental correlations used in this study.

Stephan and Abdelsalam (1980) correlation got the lowest OAD and the most centered on 0 OD. However, it was Gorenflo and Kenning (2010) correlation that had most data inside a 30% error interval even though the OAD was the highest.

Table 3.6 – OAD, OD, and γ_{30} results using pure component correlations and PR for copper heater

Correlation	Copper						
Parameter	OAD	OD	γ_{30}				
h_{SA}	0.342	-0.0541	0.531				
h_C	0.438	-0.136	0.375				
h_{RJ}	0.385	0.113	0.606				
h_G	0.443	0.251	0.614				
h_{Li}	0.348	-0.116	0.490				

3.1.1.6 Summary

For the following data analysis, a decision needs to be made regarding which pure correlation to use. Ribatski and Jabardo (2003) correlation performed better overall and in several specific parameters for our fuel heater application. However, it had poor performance on one of the specific parameters for fuel heater that was high reduced pressure, Gorenflo and Kenning (2010) was the only correlation to predict accurately on high reduced pressure. So both of these correlations were assessed for mixture and fuel data, and consequently high reduced pressure HTC predictions.

Table 3.7 shows the best correlation for a pure component as a function γ_{30} . Ribatski and Jabardo (2003) correlation is the most present, covering areas like the nature of the component and overall. But, we can not neglect the results for higher pressures achieved by Gorenflo and Kenning (2010) correlation. Both of these correlations are used in further analysis.

Parameter	Best correlation
Overall	Ribatski and Jabardo (2003)
Hydrocarbon	Ribatski and Jabardo (2003)
Alcohol	Ribatski and Jabardo (2003)
Low-pressure	Ribatski and Jabardo (2003)
Middle-pressure	Gorenflo and Kenning (2010)
High-pressure	Gorenflo and Kenning (2010)
Horizontal tube	Ribatski and Jabardo (2003)
Wire and platinum	Gorenflo and Kenning (2010)
Copper	Gorenflo and Kenning (2010)

Table 3.7 – Summary of the pure component data analysis focused on fuel heating applications

3.1.2 Binary Mixture

From the 6621 points, 3093 are from binary mixtures. The removed data due to instabilities, or lack of components on Multiflash, was different for the three EOS. The data for CPA is 2885 points, PR is 2765, and SRK is 2900 points. Comparing the three datasets of each EOS, we have 2714 points to analyze. There were no pure component fluid data for several mixture components. If only the mixture with components that had pure data available were used, we would have only 1555 points.

Figure 3.5 shows how the data is divided into mixtures, heater material and geometry, and reduced pressure. Just like with pure component data, refrigerant substances dominate the data, four out of five of the mixtures with more points are composed only of refrigerants. Related to materials, copper has more data points, and there are no data for brass and carbon steel. In contrast with the pure component data, the flat surface is the heater geometry with more data, more than half of the 2714 points. Using weighted molar composite average critical pressure

$$P_{pc} = \sum_{i}^{n} y_i P_c, \tag{3.3}$$

we get the data distribution that is shown on figure 3.5 for reduced pressure. Although the data is concentrated on the lower reduced pressures, we have data closer to $P_r = 1$, around 0.91 for R-22 and R-114.

3.1.2.1 Overall

Table 3.8 exhibits the results of every correlation and EOS. Thome (1983) correlation had the highest OAD and the lowest γ_{30} , but it is the simplest correlation used, it only needs the boiling range temperature difference. The best one was Thome and Shakir (1987)



(d) Reduced pressure distribution

Figure 3.5 – Data type distribution according to fluid, heater material and type, and reduced pressure for binary mixture

correlation with the PR EOS, an equation with thermodynamic mixture properties parameters on it. However, the results were very close to each other and in every combination, the Overall Deviation was below 0.

Correlation	СРА			PR			SRK		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_T	0.344	-0.212	0.621	0.335	-0.201	0.611	0.343	-0.222	0.592
h_{TS}	0.309	-0.0941	0.695	0.296	-0.0802	0.704	0.295	-0.113	0.702
$h_{F,1994}$	0.319	-0.115	0.673	0.309	-0.104	0.672	0.306	-0.125	0.671
$h_{F,1997}$	0.316	-0.127	0.688	0.308	-0.118	0.677	0.309	-0.140	0.667
h_I	0.324	-0.103	0.667	0.313	-0.0915	0.673	0.309	-0.113	0.674

Table 3.8 – Overall results for CPA, PR, and SRK using the mixture correlations of section 2.2.2 for binary mixtures using Gorenflo and Kenning (2010) correlation

Although getting better results for pure component case, Ribatski and Jabardo (2003) correlation did not perform as expected when compared to Gorenflo and Kenning (2010), as it can be seen on table 3.9. There was an increase in the OAD and a decrease in OD and γ_{30} , this shows a tendency to underestimate the HTC values when equation (2.14) is used. Again, the EOS did not impact hugely on the results, and Thome (1983) mixture correlation had the worst performance. The best OAD and OD were achieved with Thome and Shakir (1987) mixture correlation, while Inoue *et al.* (1998) got the best γ_{30} .

Table 3.9 – Overall results for CPA, PR, and SRK using the mixture correlations of section 2.2.2 for binary mixtures and Ribatski and Jabardo (2003) correlation

Correlation		СРА			PR			SRK		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_T	0.435	-0.364	0.389	0.422	-0.350	0.388	0.434	-0.365	0.360	
h_{TS}	0.390	-0.269	0.461	0.374	-0.253	0.433	0.386	-0.275	0.443	
$h_{F,1994}$	0.391	-0.294	0.475	0.377	-0.279	0.476	0.386	-0.293	0.459	
$h_{F,1997}$	0.396	-0.302	0.448	0.385	-0.289	0.443	0.394	-0.305	0.418	
h_I	0.387	-0.285	0.478	0.373	-0.270	0.432	0.382	-0.284	0.474	

Figures 3.6 shows the distribution of the experimental HTC associated with its corresponding calculated value using Gorenflo and Kenning (2010) correlation for pure component and Thome and Shakir (1987) correlation. In contrast to the figures 3.3, some data is clearly out of the aggregated data. Methane and ethane, methane and propane, and methane and isobutane mixture calculated HTC is very underestimated, while isobutane and propane mixture is overestimated. Also, ammonia and water mixture are underestimated.



(b) Smaller HTC

Figure 3.6 – Comparison between the experimental HTC and calculated HTC using PR, Gorenflo and Kenning (2010) correlation for pure components, and Thome and Shakir (1987) for mixture, the black line is the optimum result and the red line is the 30% error

Figure 3.7 presents the experimental and calculated HTC. In contrast with pure correlations, mixture correlations had similar results, the differences are small between them. Another point is that on the mixtures that Thome and Shakir (1987) correlation performed badly, the other correlation did not perform well too.

3.1.2.1.1 Interpolated vs. Correlation

Another point that should be noted is the impact of using pure component correlations instead of experimental HTC. Some fluids present in mixtures had their pure component behavior available on the data, so it was possible to linear interpolate the heat flux of the data



Figure 3.7 – Comparison between the experimental HTC and calculated HTC using PR and Gorenflo and Kenning (2010) correlation for binary mixtures

to use on mixture correlations. Based on the available experimental data, we have only 1514 points.

Table 3.10 has the comparison between experimental data and pure component correlation. Gorenflo and Kenning (2010) correlation had the best results in comparison to interpolation and to Ribatski and Jabardo (2003). This is unexpected, but can be explained by the type of interpolation used and how far are the desired heat flux is to the available data.

The remainder of the binary mixture analysis is developed using only Gorenflo and Kenning (2010) correlation.

Correlation	Interpolated			(Goren	ıflo; Kennin	g, 2010)	(Ribatski; Jabardo, 2003)			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_T	0.268	-0.0567	0.667	0.254	-0.102	0.694	0.298	-0.202	0.559	
h_{TS}	0.276	0.151	0.769	0.194	0.0392	0.834	0.236	-0.0836	0.701	
$h_{F,1994}$	0.262	0.107	0.754	0.207	0.0192	0.795	0.229	-0.109	0.701	
$h_{F,1997}$	0.270	0.0870	0.766	0.205	-0.00937	0.803	0.246	-0.129	0.641	
h_I	0.268	0.123	0.743	0.214	0.0362	0.795	0.221	-0.0967	0.715	

Table 3.10 – Overall results using pure component correlations, (Gorenflo; Kenning, 2010) and (Ribatski; Jabardo, 2003), or linear interpolation with PR EOS

3.1.2.2 Mixture

The mixtures of interest in this study are the ones composed of hydrocarbon and alcohol. Separating these mixtures, we have 442 data points of only Hydrocarbons and 138 binary mixtures composed of Hydrocarbon and Alcohol, which is made of only Methanol and Benzene mixture.

Table 3.11 shows the results for OAD, OD, and γ_{30} . The correlations for hydrocarbon mixtures did not get good results. The OAD is high for all correlations, Thome (1983) correlation being the highest, there is a tendency to underestimate and the γ_{30} is low, below 0.35 for every correlation. However, these metrics were affected by Methane's mixtures, which did not have good predictions as it is shown by figure 3.6. For Methanol and Benzene mixture, Thome and Shakir (1987) correlation got the best result in every metric, but there was a clear tendency to underestimate, which can be extended to all the other correlations.

The results presented in this section are affected by a lack of diversity, hydrocarbon and alcohol mixture, and strong errors by Methane mixtures.

Table 3.11 – OAD, OD, and γ_{30} results for hydrocarbon and alcohol binary mixture using Gorenflo and Kenning (2010) correlation for pure component, PR, and mixture correlations

Correlation	Hy	drocarbo	ons	Hydrocarbon + Alcohol			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_T	0.775	-0.526	0.178	0.270	-0.269	0.457	
h_{TS}	0.728	-0.470	0.343	0.181	-0.171	0.848	
$h_{F,1994}$	0.732	-0.461	0.262	0.222	-0.218	0.609	
$h_{F,1997}$	0.748	-0.435	0.232	0.245	-0.241	0.5	
h_I	0.727	-0.449	0.309	0.210	-0.205	0.746	

3.1.2.3 Pressure

To analyze the pressure influence, we divided the dataset into 3 reduced pressure intervals, the same that was used for pure components. With this division, we have 1378 data points for low range reduced pressure, 1245 for middle range reduced pressure, and 91 for high range reduced pressure. Just like on the pure component dataset, there are a few data points for reduced pressure beyond 0.5.

Table 3.12 shows the data for OAD, OD, and γ_{30} in every reduced pressure range and for every mixture correlation using PR EOS and Gorenflo and Kenning (2010) pure component correlation. On low-range reduced pressures, Thome and Shakir (1987) correlation performed better with the lowest OAD, the closest to 0 OD, and the highest γ_{30} . On middle range reduced pressures, there is a change in the best correlation, Fujita and Tsutsui (1997) correlation got the best accuracy metrics. Besides being the worst correlation on the other pressure range, Thome (1983) achieved the lowest OAD and a low tendency to underestimate the HTC, but the best γ_{30} was Fujita and Tsutsui (1994) correlation. On high reduced pressures, the correlation that required mixture properties, equations (2.25) and (2.27), got the two biggest OAD, but both performed better on low and middle reduced pressure ranges.

Table 3.12 – OAD, OD, and γ_{30} results for binary mixtures in pressures interval, [0, 0.1[, [0.1, 0.5[and [0.5, 1[using Gorenflo and Kenning (2010) correlation for pure component, PR EOS, and mixture correlations

Correlation	$0 < P_r < 0.1$			0.1	$0.1 \le P_r < 0.5$			$0.5 \le P_r < 1$		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_T	0.417	-0.347	0.476	0.254	-0.0493	0.747	0.201	-0.0687	0.780	
h_{TS}	0.365	-0.254	0.584	0.220	0.0857	0.830	0.297	0.276	0.791	
$h_{F,1994}$	0.385	-0.297	0.542	0.228	0.0877	0.807	0.252	0.202	0.802	
$h_{F,1997}$	0.389	-0.308	0.526	0.217	0.0605	0.838	0.340	0.329	0.758	
h_I	0.381	-0.288	0.559	0.241	0.106	0.791	0.248	0.181	0.780	

3.1.2.4 Heater geometry

Just like on pure components, the geometries of interest are horizontal tubes and wire. For horizontal tubes, we have 135 points and 765 for wire.

Table 3.13 has the results for horizontal tube and wire using mixture correlations, PR EOS and Gorenflo and Kenning (2010) correlation. Fujita and Tsutsui (1994) has the best OAD and γ_{30} for horizontal tube between the analyzed correlations. Although Thome (1983) correlation did not have either the worst or best OAD, it had the least amount of HTC inside the

Table 3.13 – OAD, OD, and γ_{30} results for binary mixtures with horizontal tube and wire heater geometry using Gorenflo and Kenning (2010) correlation for pure component, PR EOS, and mixture correlations

Correlation	Horizontal tube			Wire		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_T	0.369	-0.0455	0.615	0.299	-0.293	0.639
h_{TS}	0.412	0.325	0.659	0.186	-0.148	0.839
$h_{F,1994}$	0.357	0.200	0.681	0.215	-0.180	0.791
$h_{F,1997}$	0.441	0.360	0.644	0.211	-0.190	0.803
h_I	0.357	0.181	0.659	0.219	-0.174	0.782

30 % error range, but it also had the most centered OD. For wire, we see the trend of Thome (1983) correlation deviating from the other mixture correlations. Thome and Shakir (1987) correlation is the best on every metric, but it is not distant to the others, with the higher distance on OAD being 0.033 and on γ_{30} 0.057.

3.1.2.5 Heater material

For heater material, we encounter the same problem found on pure component analysis, wire geometry data is composed of only one material, platinum. So from the materials of interest, copper, and platinum, the latter is already analyzed. We have 1875 data points for copper.

Table 3.14 has the results for copper heater material using mixture correlations, PR EOS and Gorenflo and Kenning (2010) correlation. The OAD results are close to each other, the biggest difference is only 0.007. However, Thome (1983) correlation has underestimated more than the other correlation and has fewer data inside the 30 % error range. Thome and Shakir (1987) correlation has a higher γ_{30} but only 0.051 distant from the lowest value.

Table 3.14 – OAD, OD, and γ_{30} results for binary mixtures with copper heater	material	using
Gorenflo and Kenning (2010) correlation for pure component, PR I	EOS, and	mix-
ture correlations		

Correlation	Copper			
Parameter	OAD	OD	γ_{30}	
h_T	0.346	-0.155	0.614	
h_{TS}	0.339	-0.0412	0.665	
$h_{F,1994}$	0.342	-0.0592	0.642	
$h_{F,1997}$	0.344	-0.0764	0.643	
h_I	0.346	-0.0445	0.646	

3.1.2.6 Summary

Table 3.15 shows a summary of the best correlation on the specific situation under fuel heating applications. Between the accuracy metrics, we gave preference to γ_{30} due to its representation of more points inside an error range. There is a clear predominance of Thome and Shakir (1987) correlation, followed by Fujita and Tsutsui (1994). But, as it was seen in the previous sections throughout the analysis, the mixture correlations return results close to each other. The biggest factor for a real change in results was the pure correlation used.

Parameter	Best correlation	
Overall	Thome and Shakir (1987)	
Pure correlation	Gorenflo and Kenning (2010)	
Hydrocarbon	Thome and Shakir (1987)	
Hydrocarbon + Alcohol	Thome and Shakir (1987)	
Low-pressure	Thome and Shakir (1987)	
Middle-pressure	Fujita and Tsutsui (1997)	
High-pressure	Fujita and Tsutsui (1994)	
Horizontal tube	Fujita and Tsutsui (1994)	
Wire and platinum	Thome and Shakir (1987)	
Copper	Thome and Shakir (1987)	

Table 3.15 – Summary of the binary mixture data analysis focused on fuel heating applications

3.1.3 Ternary mixture

At this point, the software Multiflash became more unstable, it did not converge for boiling temperature, returning NULL results. To calculate it, it was necessary to iterate using Excel's solver and the Boiling pressure. The solver estimated boiling temperature until it reached the boiling pressure, which was the system pressure. From 719 ternary points, we managed to retain 614 points for CPA, 619 for PR, and 632 for SRK. Comparing the three EOS, we managed to obtain 605 points that are present in every dataset.

Figure 3.8 shows how the data is divided into mixtures, heater material and geometry, and reduced pressure. The ternary mixture data is mainly composed of refrigerants, continuing the trend that more data is available for refrigerants. Again, copper is the heater material with more data, however, there is no data for platinum. For ternary, flat surface and horizontal tube are the only heater types presented in the gathered data. Just like binary mixture and pure component boiling, the data is concentrated on lower reduced pressure levels, the
highest value is 0.652 for R-125, R-143a, and R-134a. Interestingly, there are more points for the reduced pressure interval of [0.6, 0.7] than from 0.2 to 0.6

3.1.3.1 Overall

Table 3.16 shows the results for the correlations and EOS in estimating the HTC using Gorenflo and Kenning (2010) pure component correlation. For OAD and OD, Thome and Shakir (1987) got the best results, but for γ_{30} , Fujita and Tsutsui (1997) was better. Both of these last correlations are more complicated to use than the others because they demand properties from the mixture.

Table 3.16 – Overall results for CPA, PR, and SRK using the mixture correlations of section2.2.2 for ternary mixtures and Gorenflo and Kenning (2010) correlation.

Correlation	CPA				PR			SRK		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_T	0.415	-0.291	0.534	0.426	-0.301	0.506	0.435	-0.350	0.450	
h_{TS}	0.357	-0.0825	0.588	0.353	-0.0894	0.587	0.340	-0.149	0.575	
$h_{F,1994}$	0.382	-0.132	0.592	0.385	-0.141	0.585	0.365	-0.189	0.572	
$h_{F,1997}$	0.367	-0.127	0.602	0.372	-0.141	0.598	0.368	-0.189	0.582	
h_I	0.398	-0.117	0.562	0.399	-0.126	0.560	0.373	-0.173	0.554	

Table 3.17 shows the results using Ribatski and Jabardo (2003) correlation. The accuracy metrics are more precise using Ribatski and Jabardo (2003) correlation when combined with PR, it has a lower OAD of approximately 0.05 and a higher γ_{30} of around 0.05 in all mixture correlations and PR with exception from Thome (1983) correlation.

From this point, every ternary mixture analysis is conducted using Ribatski and Jabardo (2003) correlation due to its better overall performance.

Figures 3.9 shows the distribution of the experimental HTC associated with its corresponding calculated value using Ribatski and Jabardo (2003) correlation for pure component

Table 3.17 – Overall results for CPA, PR, and SRK using the mixture correlations of section2.2.2 for ternary mixtures and Ribatski and Jabardo (2003) correlation.

Correlation	СРА				PR	SRK			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_T	0.414	-0.354	0.512	0.421	-0.373	0.504	0.438	-0.411	0.456
h_{TS}	0.320	-0.0795	0.621	0.304	-0.0987	0.640	0.314	-0.149	0.626
$h_{F,1994}$	0.350	-0.196	0.574	0.334	-0.215	0.620	0.340	-0.251	0.610
$h_{F,1997}$	0.357	-0.168	0.588	0.339	-0.195	0.656	0.348	-0.231	0.620
h_I	0.343	-0.185	0.559	0.327	-0.203	0.615	0.331	-0.239	0.607



(d) Reduced pressure distribution

Figure 3.8 – Data type distribution according to fluid, heater material and type, and reduced pressure for ternary mixture



(b) Smaller HTC

Figure 3.9 – Comparison between the experimental HTC and calculated HTC using PR, Ribatski and Jabardo (2003) correlation for pure components and Thome and Shakir (1987) for ternary mixture, the black line is the optimum result and the red line is the 30% error

and Thome and Shakir (1987) correlation. The mixtures with ethanol or water were underestimated, while Isobutane, R-134a and Propane mixture has a cluster of overestimated values.

Figure 3.10 shows the comparison between calculated and experimental HTC for ternary mixtures using the other correlations. Again, the results are very similar. Some noticeable differences are the R-32, R-125 and R134a mixture with overestimated points for Fujita and Tsutsui (1994) correlation and R-134a, R-142b and R123 mixture calculated HTC inside the 30% red line and the black line for Fujita and Tsutsui (1994) correlation



Figure 3.10 – Comparison between the experimental HTC and calculated HTC, using PR and Ribatski and Jabardo (2003) correlation, for ternary mixtures

3.1.3.2 Mixture

There is only one mixture that is made of hydrocarbon, Propane, Isobutane, and N-Butane, which accounts for only 26 points. There is no mixture of hydrocarbon and alcohol.

Table 3.18 shows the results for the hydrocarbon mixture using Ribatski and Jabardo (2003) correlation and PR EOS. Inoue *et al.* (1998) correlation had the best OAD and γ_{30} , while Fujita and Tsutsui (1994) correlation had the same result for γ_{30} , 0.769. Correlations with similar structures, Fujita and Tsutsui (1997) and Thome and Shakir (1987) correlation, which implement mixture properties, and Fujita and Tsutsui (1994) and Inoue *et al.* (1998) correlation, which have heat flux dependency, had similar results. Also Thome (1983) correlation had the worst result for OAD and OD, it underestimated the HTC but did not have the lowest γ_{30} .

Correlation	Hydrocarbon (Propane+Isobutane+N-Butane)								
Parameter	OAD	OD	γ_{30}						
h_T	0.244	-0.385	0.577						
h_{TS}	0.0960	-0.00789	0.5						
$h_{F,1994}$	0.0941	0.00629	0.769						
$h_{F,1997}$	0.120	-0.0119	0.577						
h_I	0.0927	-0.00927	0.769						

Table 3.18 – OAD, OD, and γ_{30} results for hydrocarbon mixture using Ribatski and Jabardo (2003) correlation for pure component, PR EOS and mixture correlations

Table 3.19 – OAD, OD, and γ_{30} results for ternary mixtures in pressures interval, [0, 0.1[, [0.1, 0.5[and [0.5, 1[using Ribatski and Jabardo (2003) correlation for pure component, PR and mixture correlations

Correlation	$0 < P_r < 0.1$			0.	$1 \le P_r < 0$	$0.5 \le P_r < 1$			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_T	0.635	-0.607	0.260	0.251	-0.184	0.719	0.527	-0.527	0.05
h_{TS}	0.434	-0.205	0.343	0.204	-0.00794	0.882	0.305	-0.254	0.4
$h_{F,1994}$	0.547	-0.451	0.295	0.170	-0.0261	0.894	0.331	-0.331	0.2
$h_{F,1997}$	0.505	-0.407	0.386	0.213	-0.0300	0.879	0.298	-0.228	0.4
h_I	0.545	-0.441	0.295	0.158	-0.0118	0.888	0.345	-0.344	0.15

3.1.3.3 Pressure

For pressure, there is lack of high reduced pressure data too. The division in pressure intervals results in 254 points for [0, 0.1[, 331 points for [0.1, 0.5[and 20 points for [0.5, 1[. Most of the data for middle range reduced pressure is inside of [0.1, 0.2]. And for the high reduced pressure range, the data is composed of only one mixture, R-32, R-125, and R-134a.

Table 3.19 shows the results for ternary mixtures divided in pressure ranges using Ribatski and Jabardo (2003) correlation for pure component, PR, and mixture correlations. For low reduced pressures, the high OAD, the OD distance from zero, and the low γ_{30} can be linked to the number of points below the minus 30 % error line found on HTC distribution between experimental and calculated. Thome and Shakir (1987) correlation had the best results for OAD and OD, but Fujita and Tsutsui (1997) correlation had the best γ_{30} . On middle range reduced pressure, the correlations get more accurate with all γ_{30} bigger than 0.7 and OAD lower than 0.3. The best correlation was Fujita and Tsutsui (1994) correlation with the smallest OAD and the biggest γ_{30} . For high pressure, the best correlation was Fujita and Tsutsui (1997) correlation with the lowest OAD, most centered OD, and the highest γ_{30} .

3.1.3.4 Heater geometry

For heater geometry, we have only two geometries, horizontal tube, and flat surface, with 246 and 359 data points, respectively. Table 3.20 shows the results according to the heater geometry for ternary mixtures using Ribatski and Jabardo (2003) correlation for pure component, PR EOS, and mixture correlations. Just like the low-pressure accuracy metrics, the horizontal tube is also affected by the strong errors from water, ethylene glycol, and diethylene glycol; water, monoethanolamine, and diethanolamine; ethanol, ethylene glycol, and diethylene glycol. The best correlation for the horizontal tube was Thome and Shakir (1987) correlation with the lowest OAD, the highest γ_{30} and the closest OD to zero. For flat surface, the best γ_{30} is found on Fujita and Tsutsui (1994) correlation. This correlation does not have the best OAD, but it is very close to 0.157 achieved by Inoue *et al.* (1998) correlation.

Table 3.20 – OAD, OD, and γ_{30} results for ternary mixtures with horizontal tube and flat surface heater geometry using Ribatski and Jabardo (2003) correlation for pure component, PR and mixture correlations

Correlation	Ho	rizontal t	ube	Flat surface			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_T	0.717	-0.717	0.102	0.219	-0.138	0.780	
h_{TS}	0.419	-0.316	0.378	0.225	0.0501	0.819	
$h_{F,1994}$	0.580	-0.552	0.187	0.165	0.0162	0.916	
$h_{F,1997}$	0.546	-0.466	0.289	0.197	-0.00955	0.908	
h_I	0.575	-0.551	0.183	0.157	0.0351	0.911	

3.1.3.5 Heater material

From the heater materials of interest, only copper was present in the ternary mixture data, only 360 data points. Table 3.21 has the accuracy metrics for ternary mixtures with copper heater material, using Ribatski and Jabardo (2003) correlation for pure component, PR, and mixture correlations. All the best accuracy metrics are scattered between the mixture correlations. But we can declare Fujita and Tsutsui (1994) correlation as the best because it has the highest γ_{30} , and its OAD is distant only 0.011 from the best one 0.170.

3.1.3.6 Summary

Table 3.22 shows a summary of the best correlation on the specific situation under fuel heating applications for a ternary mixture. In this case, the correlation with better results over several specific conditions is Fujita and Tsutsui (1997) correlation. In contrast with the

Table 3.21 – OAD, OD, and γ_{30} results for ternary mixtures with copper heater material using Ribatski and Jabardo (2003) correlation for pure component, PR EOS and mixture correlations

Correlation	Copper					
Parameter	OAD	OD	γ_{30}			
h_T	0.266	-0.205	0.689			
h_{TS}	0.215	-0.0113	0.844			
$h_{F,1994}$	0.181	-0.0367	0.850			
$h_{F,1997}$	0.221	-0.0344	0.847			
h_I	0.170	-0.0247	0.842			

binary mixture data analysis, Thome and Shakir (1987) correlation was the best one only for horizontal tubes.

	Table 3.22 – Summa	ary of the ternar	y mixture data	analysis focused	on fuel	heating applica	tions
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Parameter	Best correlation
Overall	Fujita and Tsutsui (1997)
Hydrocarbon	Inoue <i>et al.</i> (1998)
Low-pressure	Fujita and Tsutsui (1997)
Middle-pressure	Fujita and Tsutsui (1994)
High-pressure	Fujita and Tsutsui (1997)
Horizontal tube	Thome and Shakir (1987)
Copper	Fujita and Tsutsui (1994)

3.1.4 Quaternary mixture

The data for the quaternary mixture has only 28 points and is from one mixture: Methane, Ethane, Propane, and Isobutane; with a flat surface copper heater at $P_r = 0.0282$. The lack of data creates a bias according to how the model will react to only one mixture. Table 3.23 shows the results for the correlations and EOS in estimating the HTC. All the correlations performed poorly, all the data is out of the γ_{30} range, and the predictions were underestimated. However, the mixture here has the same components that did not have great results in a binary mixture, methane, ethane, and propane.

Figure 3.11 shows the distribution of the experimental HTC associated with its corresponding calculated value using Gorenflo and Kenning (2010) correlation for pure component and Thome and Shakir (1987) correlation. The figure corroborates with the results shown in table 3.23, the predictions are far apart from the black and red lines. Although the calculated HTCs increase with the experimental ones, they are still underestimated.

Correlation	СРА				PR		SRK		
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	OAD	OD	γ_{30}
h_T	0.908	-0.908	0	0.908	-0.908	0	0.908	-0.908	0
h_{TS}	0.891	-0.891	0	0.891	-0.891	0	0.892	-0.892	0
$h_{F,1994}$	0.885	-0.885	0	0.885	-0.885	0	0.885	-0.885	0
$h_{F,1997}$	0.904	-0.904	0	0.904	-0.904	0	0.904	-0.904	0
h_I	0.877	-0.877	0	0.877	-0.877	0	0.877	-0.877	0

Table 3.23 – Overall results for CPA, PR, and SRK using the mixture correlations of section 2.2.2 for quaternary mixture



Figure 3.11 – Comparison between the experimental HTC and calculated HTC using PR, Gorenflo and Kenning (2010) correlation for pure components and Thome and Shakir (1987) for quaternary mixture, the black line is the optimum result and the red line is the 30% error

Just like Thome and Shakir (1987) correlation, the other four correlations could not get results inside the γ_{30} and underestimated the HTC, as shown in figure 3.12.

3.2 Gasoline

Oliveira (2017) performed experiments for gasoline, ethanol, and blends. His data were used to compare the combinations of EOS and correlations, just like in the previous section. The data gathered is composed of 105 points for 4 pressure levels: 1.02, 2.02, 3.03, and 4.03 bar. The heater is a platinum wire with $R_a = 0.3 \mu m$.

To model gasoline, Netto *et al.* (2022) gasoline surrogate for pool boiling is used with adaptations, the components, molar composition, and critical point are shown in table 3.24. On Multiflash, there is no 2,3-dimethyl pentane, so it was made a substitution, it was



Figure 3.12 – Comparison between the experimental HTC and calculated HTC, using PR and Gorenflo and Kenning (2010) correlation, for quaternary mixtures

used 3,3-dimethyl pentane, which has 29.46 *bar* and 263.3 $^{\circ}C$ as the critical point and the same molecular weight.

Table 3.25 shows the accuracy metrics when using PR EOS, and Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) correlation for pure components. Equation (2.14) predicted better than (2.16), with a tendency to underestimate the HTC. This results confirm Ribatski and Jabardo (2003) correlation better performance on hydrocarbon, however, it should be noted that the parameter f_w from equation (2.14) for platinum was determined using the same data, so there can be a bias. Thome (1983) has the worst data between the mixtures correlation, while Inoue *et al.* (1998) correlation kept the lowerest OAD and all the points inside a 30% error interval.

Component	Molar composition	$P_c(bar)$	$T_c(^{\circ}C)$
N-butane	0.04	37.96	152.0
N-pentane	0.198	33.67	196.6
N-hexane	0.138	30.18	234.7
2,3-dimethylpentane	0.176	29.2	264
2,2,4-trimethylpentane	0.388	25.70	270.7
1,2,4-trimethylbenzene	0.06	32.32	376

Table 3.24 – Netto *et al.* (2022) gasoline surrogate for pool boiling

Table 3.25 – OAD, OD, and γ_{30} results for gasoline using PR EOS and comparing Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) correlation

Correlation	Gorenf	lo and Ke	enning (2010)	Ribatski and Jabardo (2003)			
Parameter	OAD	OD γ_{30}		OAD	OD	γ_{30}	
h_T	0.228	0.0318	0.686	0.185	-0.142	0.771	
h_{TS}	0.183	0.149	0.771	0.121	-0.0476	0.981	
$h_{F,1994}$	0.161	0.149	0.8	0.0972	-0.0490	1.0	
$h_{F,1997}$	0.179	0.109	0.771	0.136	-0.0797	0.990	
h_I	0.175	0.173	0.8	0.0813	-0.0320	1.0	

Figure 3.13 show the HTC distribution between experimental and calculated ones using Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) correlation, and Inoue *et al.* (1998) correlation, figures 3.13a and 3.13b, respectively. These graphs show how the correlations start to deviate from the optimum value as the experimental HTC get bigger, the effect is more intense for equation (2.16), and equation (2.14) keeps the data inside the 30 % range. At lower values of HTC, both correlations were able to keep the data inside the error range, with Gorenflo and Kenning (2010) correlation more prone to overestimate the HTC.

3.3 Ethanol-gasoline blend

Again, Oliveira (2017) experimental data were used for comparison. His ethanol/gasoline blend data is composed of E35, E50, E65, E80, and E90 blends, where "E" represents ethanol, and the number that follows is the percentage of ethanol in the mixture. The experiments were made on pressures of 1.02, 2.02, and 4.03 bar, with the same heater as the gasoline data.

For blends, we found difficulty with vapor-liquid equilibrium on Multiflash. The software could not form a stable solution with only two phases when we used PR EOS. It was necessary to appoint a third phase, a liquid one, but this changes the calculation from VLE to vapor-liquid-liquid-equilibrium, which is not our case and ethanol is miscible with gasoline. So we changed to CPA, and from there on it managed to form a stable solution with vapor and



Figure 3.13 – Comparison between the experimental HTC and calculated HTC for gasoline using different pure component correlations, PR and Inoue *et al.* (1998) mixture correlation

liquid phases. CPA is an EOS created to deal better with hydrate inhibitors like methanol, so it works better with associative fluids like ethanol.

Table 3.26 shows the results - OAD, OD, and γ_{30} - for blends using CPA, mixture correlations, and equations (2.16) and (2.14) for the pure part. Clearly, Ribatski and Jabardo (2003) correlation had the best predictions, it kept in every mixture correlation more than 0.9 on γ_{30} and OAD lower than 0.11. Although being constantly the worst mixture correlation on several occasions, Thome (1983))'s correlation got the best metrics in both cases. The other mixture correlations were packed together with no difference being bigger than 0.114 between the metrics.

Table 3.26 – OAD, OD, and γ_{30} results for blends using PR EOS and comparing Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) correlation

Correlation	Gorent	lo and K	Cenning (2010)	Ribatski and Jabardo (2003)			
Parameter	OAD	OD	γ_{30}	OAD	OD	γ_{30}	
h_T	0.292	0.287	0.592	0.0775	0.0220	0.969	
h_{TS}	0.356	0.356	0.404	0.104	0.0710	0.929	
$h_{F,1994}$	0.332	0.332	0.439	0.0890	0.0547	0.957	
$h_{F,1997}$	0.313	0.311	0.518	0.0857	0.0393	0.961	
h_I	0.351	0.351	0.416	0.0937	0.0680	0.945	

Figure 3.14 show the experimental and calculated HTC distribution using Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation, CPA and Inoue *et al.* (1998) mixture correlation. Gorenflo and Kenning (2010) correlation usually



Figure 3.14 – Comparison between the experimental HTC and calculated HTC for ethanol and gasoline blends using different pure component correlations, CPA and Inoue *et al.* (1998)

overestimates the HTC, and has its calculated HTC around the line of 30% error, as the HTC increases, the data becomes more dispersed and separate from the red line. In contrast, Ribatski and Jabardo (2003) has most of its data inside the 30% error interval, with a few HTC being overestimated. There is a concentration of HTC over the black line, which is the optimum result. The results shown here contribute to what is present in table 3.26

The pure component correlations used show a bigger impact on the final HTC than the EOS and the mixture correlations. The mixture correlations, except for Thome (1983), had similar results in almost every specific situation and overall analysis. Only a few cases the difference between the metrics was bigger than 0.1.

The EOSs were not a decisive factor in the results until the blend fuel analysis. On all the other occasions, PR and SRK were able to form stable solutions with two phases, liquid, and vapor.

For the following sections of chapter 3, predictions were made based on what was evaluated in section 3.1. The EOS used is CPA, because it is the one that worked on every occasion. Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) correlation will be used combined with Thome and Shakir (1987) correlation.

3.4 High reduced pressure HTC prediction

At this point, we pass to estimating the HTC at high pressure for ethanol, gasoline, and blends, E35, E50, and E90, from pressure 1 bar to 25 *bar* for gasoline and blends, and 1 to 60 bar - 0.015 to 0,96 of reduced pressure - for ethanol. It was analyzed the impact of increasing pressure with constant heat flux and the impact of increasing heat flux at constant pressure. The heat fluxes used for increasing pressure will vary according to the mixture and its critical heat flux, which is calculated by using the mixture properties on equation (2.29) (Gorenflo; Kenning, 2010). The heater is a platinum wire with $R_a = 0.3 \mu m$. The correlation used for comparison are Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) for pure component and Thome and Shakir (1987) for mixture. And the EOS is CPA.

The gasoline's surrogate critical point is 31.77 bar and $258.03 \circ C$ and 2,2,4-trimethyl pentane has a critical pressure of $25 \ bar$. This creates a problem related to the ideal heat transfer coefficient model. When dealing with mixtures that have one component beyond its pure critical point, there is not a pure component pool boiling equivalent at the same pressure as the mixture. For example, in our case, if the gasoline is at 26 bar, it is possible to calculate a pure component nucleate pool boiling HTC at 26 bar for only 5 components that still face a phase change. 2,2,4-trimethyl pentane do not have an equivalent, and this is not covered by the ideal HTC. One of the possibilities would be to use an HTC from natural convection, but this kind of HTC is usually orders of magnitude below pool boiling HTC. The same situation is present for blends, and it gets worse because the ethanol critical pressure is 62 bar.

Also, Multiflash Software had problems converging with E90 at certain pressures. This issue was not seen on other blends.

3.4.1 Ethanol

Figure 3.15 shows the CHF for ethanol as a function of pressure. At lower pressures the CHF increases until it reaches a peak of 934 kW/m^2 at 17 bar, 0.27 reduced pressure, then it starts to decrease. Close to the critical pressure, the CHF goes to zero, because the vaporization enthalpy, the surface tension, and the difference between liquid and gas density approximates to zero as the pressure increase.

Figure 3.16 shows the HTC using either Ribatski and Jabardo (2003) or Gorenflo and Kenning (2010) correlations at different pressures, 1, 17, 34 and 60 bar, with increasing heat flux from 1 kW/m^2 until its corresponding CHF at that pressure level. On all pressure



Figure 3.15 – Ethanol critical heat flux according to pressure

levels, as the heat flux gets higher, the larger the difference between the two correlations, and the difference increase with the pressure, achieving more than $150 \ kW/m^2/K$ on 60 bar. That is a behavior that was first seen on the pure component data analysis, where Gorenflo and Kenning (2010) correlation got higher HTC for higher pressures. This increase might not be beneficial for Gorenflo and Kenning (2010) correlation at lower pressures, but it is necessary to further compare between pool boiling HTC correlations with high-pressure experimental data.

Figure 3.17 shows another kind of analysis, keeping the heat flux constant and increasing the pressure for both Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) correlation. Some of the heat fluxes do not comprise the whole pressure range because they are only feasible on certain pressures. The heat fluxes that are capable of getting to higher pressures, 100 and 350 kW/m^2 , show a rapid increase on HTC at higher pressures. For 100 kW/m^2 , the increasing is the fastest between the other evaluated heat fluxes, passing the 200 $kW/m^2/K$ level, if using Gorenflo and Kenning (2010) correlation. It is interesting to note that at 100 kW/m^2 the HTC might achieve the same HTC as the 850 $kW/m^2/K$ but at the cost of doubling the working pressure.

Although similar in shape, the values of HTC are far apart between the two correlations. Again, Gorenflo and Kenning (2010) had the highest HTC values.

3.4.2 Gasoline

From there on, a mixture correlation is used for gasoline and ethanol-gasoline blends. The chosen one is Thome and Shakir (1987) correlation.



Figure 3.16 – HTC for ethanol at different pressure using CPA, Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation

Although not able to calculate the HTC near gasoline's critical point due to the nonexistence of boiling phenomenon on 2,2,4-trimethylpentane beyond 25.7 bar, it is possible to determine its CHF until the critical point. Figure 3.18 shows the CHF as a function of pressure. It has a similar behavior as ethanol CHF, but with lower values. The maximum CHF of 485.3 kW/m^2 occurs at 9 bar.

Figure 3.19 shows the HTC at different pressures with variable heat flux using Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation, Thome and Shakir (1987) mixture correlation, and CPA. Despite the high difference between the pure component correlations found on ethanol, for gasoline, the difference is smaller. It increases until 20 bar, but at 25 bar, it decreases. The linear behavior persists as the heat flux increases.

Figure 3.20 shows the behavior of HTC at different heat flux levels according to the pressure for gasoline with different pure component correlations, Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003). As the pressure increases, the HTC does too, but again, the higher heat flux impacts more than increasing the pressure. Pressure increase did not manage



(b) Ribatski and Jabardo (2003)

Figure 3.17 – HTC behavior for constant heat flux according to pressure for ethanol using CPA and different pure component correlation

to get HTC similar to heat flux increase at middle range pressures. However, the problem stated before about the impossibility of reaching around the critical pressure impedes the analysis of HTC beyond 25 bar.

3.4.3 Blend

Based on equation (2.29), we get the figure 3.21 that shows the CHF for E35, E50, and E90 according to pressure until near the critical pressure. Increasing the amount of ethanol in the mixture, elevates the maximum CHF, passing from 622.2 kW/m^2 on E35 to 840 kW/m^2 on E90, with the same maximum pressure. For E50, the max CHF is 638.6 kW/m^2 at 13 bar. All of these values are higher than the ones predicted for gasoline but lower than for ethanol.

Figure 3.22 shows the HTC at different pressures with variable heat flux using Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation, Thome and Shakir (1987) mixture correlation, and CPA for E35. The results and behavior of



Figure 3.18 - Gasoline's surrogate critical heat flux according to pressure



Figure 3.19 – HTC for gasoline at different pressure using CPA, Thome and Shakir (1987) mixture correlation and Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation

HTC are similar to gasoline, the pure component correlation predicts close values, with a difference lower than 30 %. On higher heat fluxes the HTC behaves linearly, in contrast with low heat flux, where there is a gradient variation.

Figure 3.23 shows the HTC at different pressures with variable heat flux using



(b) Ribatski and Jabardo (2003)

Figure 3.20 – HTC behavior for constant heat flux according to pressure for gasoline using CPA, Thome and Shakir (1987) mixture correlation and different pure component correlation

Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation, Thome and Shakir (1987) mixture correlation, and CPA for E50. There is a clear increase on HTC in comparison to E35 for every pressure, passing from 5.7 $kW/m^2/K$ for E35 on 1 bar for Gorenflo and Kenning (2010) correlation to 7.0 $kW/m^2/K$ for E50 at the same pressure and correlation. And for 25 bar, we have 17.5 $kW/m^2/K$ for E20, while 24.3 $kW/m^2/K$ for E50.

Figure 3.24 shows the HTC at different pressures with variable heat flux using Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation, Thome and Shakir (1987) mixture correlation, and CPA for E90. With this amount of ethanol, the deviations between the correlations get higher. Just like on pure ethanol, the value of h_G can make the final result double what was achieved with h_{RJ} . This mixture achieved the highest HTC in comparison to the other mixtures. And presented a similar behavior on lower heat flux,



Figure 3.21 – Blends critical heat flux according to pressure



Figure 3.22 – HTC for E35 blend at different pressure using CPA, Thome and Shakir (1987) mixture correlation and Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation

but there is not a clear linear behavior of the HTC.

Figure 3.25 shows the behavior of HTC at different heat flux levels according to the pressure for E35 with different pure component correlations, Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003), CPA and Thome and Shakir (1987) mixture correlation. Just like



Figure 3.23 – HTC for E50 blend at different pressure using CPA, Thome and Shakir (1987) mixture correlation and Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation

in other cases, the HTC increases with the pressure, but with less intensity than for gasoline and ethanol. E35 has a higher critical pressure than gasoline, so the effect of not being able of calculating beyond 25 bar harm the analysis. Gorenflo and Kenning (2010) correlation has higher HTC than Ribatski and Jabardo (2003) correlation.

Figure 3.26 shows the behavior of HTC at different heat flux levels according to the pressure for E50 with different pure component correlations, Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003), CPA and Thome and Shakir (1987) mixture correlation. E50 has a similar behavior to E35 but with a higher increase of HTC and a stronger limitation of further analysis, because the critical pressure increase, and the model only reach 25 bar. Higher amounts of ethanol contribute to a better HTC and a broader spectrum of pressure at each heat flux.

Figure 3.27 shows the behavior of HTC at different heat flux levels according to the pressure for E90 with different pure component correlations, Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003), CPA and Thome and Shakir (1987) mixture correlation. This



Figure 3.24 – HTC for E90 blend at different pressure using CPA, Thome and Shakir (1987) mixture correlation and Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) pure component correlation

last blend is very close to pure ethanol, so it has a higher critical pressure and allows higher heat flux on larger pressure ranges. However, the impact of 2,2,4-trimethylpentane worsens the results. The 25 bar pressure limit is very far from ethanol's critical pressure. Again, Gorenflo and Kenning (2010) correlation has higher values in all cases, and, as it was previously seen, the difference between the results using each of the pure correlation gets higher.



Figure 3.25 – HTC behavior for constant heat flux according to pressure for E35 using CPA, Thome and Shakir (1987) mixture correlation and different pure component correlation



Figure 3.26 – HTC behavior for constant heat flux according to pressure for E50 using CPA, Thome and Shakir (1987) mixture correlation and different pure component correlation



Figure 3.27 – HTC behavior for constant heat flux according to pressure for E90 using CPA, Thome and Shakir (1987) mixture correlation and different pure component correlations

4 SUPERCRITICAL NATURAL CONVECTION

Heating at pressures higher than the critical pressure, there is no boiling, only natural convection. To model this phenomenon, in this work, we simulated the transient natural convection inside a fuel heater. The CFD result for HTC and fluid/surface temperatures were compared to the results obtained through natural convection equations suitable for concentric cylinders using the temperature average of the properties

$$j_{avg} = \frac{1}{\Delta T} \int_{T_i}^{T_f} j(T) dT$$
(4.1)

and constant properties through the film temperature. The transient numerical simulation allows the understanding of how the flow forms, the temperature reached, and how the supercritical properties variation will affect it.

Since 62.68 *bar* and 240.85 °*C* are the critical pressure and the critical temperature for ethanol, the pressures of analysis were 63, 80, 100, 200, and 1000 *bar*, which are 1.01, 1.28, 1.60, 3.20, 15.95 in reduced pressure. The temperature is set at an initial condition of 26.85 °*C*, and free to vary until it reaches the limit of Schroeder *et al.* (2014) EOS temperature interval validity upper limit, 376.85 °*C*. All pressures selected are higher than the critical pressure and represent different property behavior found for supercritical fluid, because 63, 80, and 100 *bar* properties vary intensively due to temperature changes, while 200 and 1000 *bar* behave differently. Figures 4.1, 4.2, 4.3, and 4.4 show the change of the following ethanol properties density, specific heat at constant pressure, thermal conductivity and dynamic viscosity for the working pressures in a temperature interval of 26.85 °*C* and 376.85 °*C*, which were calculated using Schroeder *et al.* (2014) EOS and CoolProp. The points indicate the reduced temperature where is the pseudocritical point based on the specific heat at constant pressure and the thermal diffusivity. As the pressure level increases, the high property variation disappear, except for the dynamic viscosity, which is still highly influenced by the temperature.

The proposed heat fluxes for analysis are 50, 100, 150, and 200 kW/m^2 . These heat fluxes are smaller than the ones used on fuel heating applications, but they allow the visualization of the supercritical effect. Another point that prevents higher heat fluxes is the temperature application range for the EOS. The final time of simulation is 4 seconds of complete heating if the fluid did not reach the upper limit temperature 376.85 $^{\circ}C$. Simulating beyond this temperature causes instability in the simulation.



Figure 4.1 – Density as a function of the temperature in different pressure levels, the point indicates the temperature that specific heat at constant pressure reaches its maximum



Figure 4.2 – Specific heat at constant pressure as a function of temperature in different pressure levels, the point indicates the temperature that specific heat at constant pressure reaches its maximum



Figure 4.3 – Thermal conductivity as a function of temperature in different pressure levels, the point indicates the temperature that specific heat at constant pressure reaches its maximum



Figure 4.4 – Dynamic viscosity as a function of temperature in different pressure levels, the point indicates the temperature that specific heat at constant pressure reaches its maximum

To conduct a transient analysis, ANSYS Fluent 19.0 simulated the natural convection inside a 2D chamber of the concentric cylinder, where the inner cylinder is the heater, and the outer one is insulated. The geometry has a relief path under the cylinder, so the pressure level is kept constant throughout the simulation. As the fluid expands, it pushes part of the fluid through the relief path until the outlet is at a fixed pressure. The size of the relief is chosen long enough so it does not influence the flow formation inside the heating chamber. The walls of the relief path are also insulated. This geometry is based on PFI Marelli's fuel heater, similar to the figure 1.3a. Figure 4.5 shows the schematic drawing of the heater and the setup of the problem. There we have the concentric cylinder, the relief, and the indications of the boundary and initial conditions for heat flux and temperature.



Figure 4.5 – Schematic drawing of the simulated geometry

The geometry and boundary conditions presented are an improvement from the used on (Morais *et al.*, 2022). The conditions of fixed heat flux and initial ambient temperature of 26.85 °*C* are closer to reality.

The system of partial differential equations solved, equations (2.33), (2.34) and (2.35), is solved with all properties, density, specific heat at constant pressure, thermal conductivity and dynamic viscosity varying. We used a second order upwind scheme for the convective terms and a first order time implicit scheme.

4.1 Mesh independence study

We studied the mesh independence by simulating the natural convection at 65 bar and heat flux of 150 kW/m^2 and analyzing the average HTC after 0.5 seconds. This pressure level has the strongest thermodynamic and transport properties variation, as can be seen in figures 4.1, 4.2, 4.3, and 4.4.

Table 4.1 shows the average HTC on the heater cylinder wall for several meshes at 65 bar and heat flux of 150 kW/m^2 at 0.5 seconds. As the number of nodes increases, the

variation between meshes just gets smaller. Comparing meshes 4 and 5, the absolute difference is only 0.57 and the relative is 0.067%, while the number of nodes more than doubled. The mesh nodes increment was focused on increasing the number of nodes near the heated wall because that is where the flow varies the most.

The final mesh has 102681 nodes with a step time of 0.0003125. To simulate the supercritical natural convection flow, it was used a workstation with a CPU Intel Xeon W-1290 and 64 GB of RAM, 10 cores were used. It took 2 days to simulate the flows with 150 kW/m^2

Table 4.1 – Average HTC on the heater cylinder wall for several meshes at 65 bar and heat flux of 150 kW/m^2 at 0.5 seconds

Mesh	Nodes	Average HTC $(W/m^2/K)$
1	30590	861.09
2	61414	851.27
3	102681	849.16
4	121590	848.98
5	243397	848.41

4.2 Transient analysis

Appendix A shows the temperature field and velocity for different moments of the simulation. These figures represent how the flow is constituted inside a concentric cylinder 2D geometry. First, there is a moment of only conduction heat transfer, then it is followed by a formation of a plume right over the heater's top. This plume moves hot fluid to the top of the geometry where the heated fluid shocks with the outer cylinder wall and then disperse on two sides. This disturbance generates vortices that affect the plume path, making it oscillatory and consequently forming more vortices. This process persists and the heat is spread across the top of the geometry. The cold fluid is pushed down and, due to the particularity of the proposed geometry, part of the fluid leaves the chamber and a bigger part is driven towards the bottom of the heater, where it is heated and continues the cycle.

The amount of oscillating effect is increased with lower pressures and higher heat flux. Nevertheless, this behavior remains at the top of the geometry.

4.2.1 Results for $q = 50 \, kW/m^2$

Figure 4.6 shows the temperature and y-velocity profiles for all the pressures at the middle of the geometry at 1, 2, 3, and 4 seconds with a heat flux of 50 kW/m^2 . For 1 and 2

seconds, the profiles are similar to each other, but at 2 seconds there is a small increment in the temperature profile. Also, only the thermal boundary layer shows signs of heat spreading to the fluid in this area. However the velocity profile is already established, showing how the fluid goes up near the wall, and the rest of the cross-section goes down. Pressures of 65, 80, 100, and $200 \ bar$ behave similarly, their lines are almost combined, and small differences can be seen in the maximum and minimum peaks. The pressure of $1000 \ bar$ is more thermal diffusive with a wider thermal boundary layer and gets lower values of y-velocity.

At 3 seconds, we see that heated fluid is convected to the lower region of the heating chamber through the combination of higher temperature fluid between the outer wall and the local minimum and the negative y-velocity. For 65, 80, 100, and 200 *bar* y-velocity profile has a convex state when it is negative, showing a more intense backward flow near the wall and between the maximum global temperature and the maximum local temperature. Also, part of the cold fluid is also being moved to the upper part of the heating chamber.

At 4 seconds, 1000 *bar* velocity profile gets more similar to the other pressure levels, but it is still more diffused in comparison to the other cases. The heated fluid is still being convected to the lower section of the geometry, and there is a clear increase in the outer wall temperature. Both sides are symmetric in all velocities.

Figure 4.7 shows the temperature profile of the plume formed above the top of the heater with a heat flux of 50 kW/m^2 at 1, 2, 3, and 4 seconds in all pressure levels. Except for 1000 *bar*, at 1 and 2 seconds, all the other temperature profiles at different pressure levels are similar. The pressure of 1000 *bar* slows down convection, at 1 second the hotter fluid leaving the heater did not reach the top of the outer cylinder.

At 3 seconds, an oscillating profile temperature is presented for 65, 80, and 100 *bar*. Ethanol at a pressure of 200 and 1000 *bar* are one over the other will no oscillating sign. At 4 seconds, the behavior continues, with 65, 80, and 100 *bar* flow propagating its oscillation, increasing the contact of colder fluid with the plume.



Figure 4.6 – Temperature and y-velocity profile in the middle of the chamber for 1, 2, 3, and 4 seconds with a heat flux of 50 kW/m^2



Figure 4.7 – Temperature profile of the plume in different moments with a heat flux of 50 kW/m^2

Figure 4.8 shows the maximum temperature on the heater wall throughout the simulation. The temperature grows fast until it reaches a plateau of around 0.75 seconds, with an exception at 1000 *bar*, which only reaches this change of behavior after 1 second. Then, at all pressures, the temperature grows with some oscillations. After 2.5 seconds, the temperature grows almost linearly. The temperature reached were not close to the critical point of 240.85 $^{\circ}C$

Figure 4.9 shows the average wall temperature at the heater cylinder for all the pressures with a heat flux of 50 kW/m^2 . Just like with maximum temperature, there is fast growth followed by stabilization, then growth at a slower velocity. The pressure that differs is 1000 *bar* which has a stabilization separated from the other pressure levels. Also, 1000 *bar* is not parallel to the other heating processes, it reached 200 *bar* HTC and then the group of pressures 65, 80, and 100 *bar* at the end of the simulation.



(a) All simulation time interval (b) Simulation time interval beyond 1 second

Figure 4.8 – Maximum temperature at the heater cylinder wall for 50 kW/m^2



Figure 4.10 shows the average HTC on the heater cylinder wall for 50 kW/m^2 . At the beginning of the simulation, there is a high peak of HTC, then followed by a continuous decrease of HTC. The pressure level of 1000 *bar* has a slower falling rate, separating it from the other pressure levels.



Figure 4.10 – Average HTC at the heater cylinder wall for 50 kW/m^2

The last part of the analysis on heat flux of 50 kW/m^2 is the temperature profile of the fluid over the heater's wall with its corresponding properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity. Figures 4.11 and 4.12 show the profiles at 1 and 4 seconds. The temperature profile shows that at the highest point of the heater occurs the highest temperature, while at the bottom there are the lowest values of temperature. At the bottom, the variation of temperature is not high, and this reflects on the properties. The differences between properties are caused by pressure. As it was seen in figure 4.10a, at 1 second, the HTC is higher for 1000 *bar*, and this is a reflection of the lower temperatures on the top of the heater in comparison to the other pressures.



Figure 4.11 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 50 kW/m^2 at 1 second over the heater surface



Figure 4.12 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 50 kW/m^2 at 4 seconds over the heater surface

4.2.2 Results for $q = 100 \, kW/m^2$

Figure 4.13 shows the temperature and y-velocity profiles at the middle of the geometry for all the pressures at 1, 2, 3, and 4 seconds with a heat flux of 100 kW/m^2 . The temperature difference between the wall temperature and the bulk fluid is bigger than on 50 kW/m^2 , achieving more than 140 °C. The temperature profile at 2 seconds has a higher local temperature peak than with 50 kW/m^2 , and this causes a lower density and a higher velocity in the velocity profile.

At 3 and 4 seconds there is a resistance to fluid motion to the lower side of the heater. The faster velocities towards the bottom are found near the insulated wall and just after
the decrease in temperature. Ethanol at a pressure of 1000 bar diffuse just like on 50 kW/m^2 , while the other pressures are packed together.



Figure 4.13 – Temperature and y-velocity profile in the middle of the chamber for 1, 2, 3, and 4 seconds with a heat flux of 100 kW/m^2

Figure 4.14 shows the temperature profile of the plume formed above the top of the heater with a heat flux of $100 \ kW/m^2$ at 1, 2, 3, and 4 seconds in all pressure levels. With 100 kW/m^2 heat flux, ethanol at 1000 bar had a temperature profile closer to the other pressures at 1 second. However, at 2 seconds, 65, 80, 100, and 200 bar are already facing an oscillatory temperature, while 1000 bar had just started to oscillate, on a small level, at 3 seconds. Also, at 2 seconds, except for 1000 bar, the lowest temperature achieved is below 75 °C. At 4 seconds, except for 1000 bar, the ethanol at different pressure levels show a similar oscillation, but apparently on a different phase. This oscillatory behavior indicates that vortices are bringing cold fluid to the plume path.



Figure 4.14 – Temperature profile of the plume in different moments with a heat flux of 100 kW/m^2

Figure 4.15 shows the maximum temperature on the heater throughout the simulation with 100 kW/m^2 . The temperature grows fast until it reaches a plateau of around 0.5 seconds, with an exception to the pressure of 1000 *bar*, which only reaches this change of behavior after 0.75 seconds. Then, in all pressures, the temperature grows with stronger oscillations than in 50 kW/m^2 . Two hundred *bar* pressure ethanol had a higher temperature than the

other pressure levels, but they remained close to each other



Figure 4.15 – Maximum temperature at the heater cylinder wall for 100 kW/m^2

Figure 4.16 shows the average wall temperature at the heater cylinder for all the pressures with a heat flux of 50 kW/m^2 . There is a fast growth followed by a less intense one, where the average temperature increased with a lower temperature variation in time. Just like with the heater's maximum temperature, at pressure of 200 *bar*, the ethanol reached the highest temperature.



Figure 4.16 – Average temperature at the heater cylinder wall for 100 kW/m^2

Figure 4.17 shows the average HTC at a heater cylinder wall for $100 \ kW/m^2$. There is a high peak at the beginning due to the high heat flux and small temperature difference. But just like the other temperature variables, average temperature and max temperature at the heater cylinder wall, the HTC stabilizes and slowly decreases. Ethanol at pressures of 65, 80, and 100 *bar* had very similar HTC decreases. And at 1000 *bar*, it is distant from the other conditions, but at 4 seconds it reaches the 200 *bar* curve, showing a smaller HTC decrease.



Figures 4.18 and 4.19 show the temperature and properties profiles at 1 and 4 seconds with heat flux of $100 \ kW/m^2$. Despite the temperature profiles being close together, the pressure difference affects the properties. Sixty-five *bar* ethanol has a specific heat at constant pressure of almost $10000 \ W/kg/K$ at 4 seconds because it is getting closer to the pseudocritical pressure. This huge value does not create an unusual behavior on the temperature profile. Some small temperature differences on the profiles exist and indicate the difference in the HTC.



Figure 4.18 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 100 kW/m^2 at 1 second over the heater surface



Figure 4.19 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 100 kW/m^2 at 4 seconds over the heater surface

4.2.3 Results for $q = 150 \, kW/m^2$

Figure 4.20 shows the temperature and y-velocity profiles at the middle of the geometry for all the pressures at 1, 2, 3, and 4 seconds with a heat flux of 150 kW/m^2 . The temperature and y-velocity profiles are similar to the ones presented before. They showed the high temperature achieved by the wall and how the flow moved heated fluids to the lower part of the heater. The difference here is the increase of the absolute values, the temperature achieves 200 °C and the highest velocity is almost 0.024 m/s. Another point is that the flux of fluid flowing to the lower part of the cylinder has a straight line varying only near the heater and the insulated outer wall. Again, at the pressure of 1000 *bar*, ethanol diffused more momentum and



Figure 4.20 – Temperature and y-velocity profile in the middle of the chamber for 1, 2, 3, and 4 seconds at 150 kW/m^2

Figure 4.21 shows the temperature profile of the plume formed above the top of the

heater with a heat flux of $150 \ kW/m^2$ at 1, 2, 3, and 4 seconds in all pressure levels. With this heat flux, the temperature profiles oscillate even more and are not restricted to the lower pressure levels evaluated. The high temperature presented achieves the pseudocritical temperature and near the wall at 1 and 2 seconds, there is a change in the temperature gradient. At this heat flux, there is no pattern of oscillation with a phase difference. It is also possible to visualize the cold fluid moved by the vortices pushing fluid to the plume and reducing its temperature at certain locations.



Figure 4.21 – Temperature profile of the plume in different moments with a heat flux of 150 kW/m^2

Figure 4.22 shows the maximum temperature on the heater throughout the simulation. Another plateau is formed, but before the temperature increase slowed down, there had been a temperature peak that is higher for lower pressures. After the peak, the temperature decreases and starts to oscillate. The three lowest pressure levels start to oscillate in a high frequency which can indicate two things, turbulence or numerical instabilities, and it is caused by the high heat flux followed by high properties variation near the pseudocritical point. These three pressure levels have pseudocritical points with strong properties variation, as shown at figures 4.1, 4.2, 4.3, 4.4. Turbulence in 2D is not an expected phenomenon, it is indicating that the model needs to be adapted to better comprise the property fluctuations. Apart from this, 65 bar pressure ethanol had the highest increase in temperature. This is explained by the low density, specific heat, and thermal conductivity after the pseudocritical point.



Figure 4.22 – Maximum temperature at the heater cylinder wall with a heat flux of $150 \ kW/m^2$

Figure 4.23 shows the average wall temperature at the heater cylinder for all the pressures with a heat flux of 150 kW/m^2 . The same behavior from the other situations is shown, however with increased oscillation for 65, 80, and 100 bar.



(a) All simulation time interval

Figure 4.23 – Average temperature at the heater cylinder wall for 150 kW/m^2

Figure 4.24 shows the average HTC at a heater cylinder wall for 150 kW/m^2 . Just like the average temperature on the heater, the HTC oscillates more, a consequence of what has been seen throughout the case with 150 kW/m^2 .



Figures 4.25, 4.26, 4.27, and 4.28 show the temperature and properties profiles over the heater at 1, 2, 3, and 4 seconds with $150 \ kW/m^2$. For 65 *bar* ethanol, as the temperature gets closer to the pseudocritical point it starts to increase slowly, and after the temperature reached it, there is a sharp increase in temperature because of the deterioration of the local HTC. At 4 seconds the pseudocritical point over the wall has moved from the center in comparison to 1 second. And another gradient discontinuity is created closer to the center, reproducing the same behavior: slow temperature increase, then sharp temperature increase. These occur because another point near the pseudocritical point is located just above the thin liquid film adjacent to the wall. Although most of the temperature of ethanol at pressure of 65 bar is lower than at pressure of 1000 *bar*, on the top of the heater at 4 seconds, the sharp temperature increase leads the heater to the highest level of temperature than the others, just like it was seen on figure 4.22. These effects were not seen on the other pressure levels.



Figure 4.25 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 150 kW/m^2 at 1 second over the heater surface



Figure 4.26 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 150 kW/m^2 at 2 seconds over the heater surface



Figure 4.27 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 150 kW/m^2 at 3 seconds over the heater surface



Figure 4.28 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 150 kW/m^2 at 4 seconds over the heater surface

4.2.4 Results for $q = 200 \, kW/m^2$

With this heat flux, $200 \ kW/m^2$, it were not possible to keep the temperature below the limit of Schroeder *et al.* (2014) equation of state throughout the whole simulation period. So, when the simulation achieved any temperature higher than the EOS, we stopped the simulation. The worst case was at 65 *bar* with only 0.254 *s* of simulation time until it achieved the temperature limit. On the other hand, at 1000 *bar*, the simulation lasted until 2.15 seconds.

Figure 4.29 shows the temperature and y-velocity profiles at the middle of the geometry for all the pressures at 0.25, 1, 1.5, and 2 seconds with a heat flux of 200 kW/m^2 . At 1, 1.5, and 2 seconds, ethanol at pressures of 65, 80, and 100 *bar* achieve a temperature higher than 376.85 $^{\circ}C$, which is outside of the EOS validity range. At 0.25 second, the profiles are similar, however, their peak values are different, with the higher the pressure, the lower the absolute peak value of temperature and y-velocity. At 1, 1.5, and 2 seconds the profile formation is similar to the other heat flux cases.

Figure 4.30 shows the temperature profile of the plume formed above the top of the heater with a heat flux of 200 kW/m^2 at 0.25, 1, 1.5, and 2 seconds in all pressure levels that are still under EOS validity. At 0.25 seconds, the lower pressure levels achieve higher temperatures with a very strong step decrease from the heater wall. In other moments, there is a strong oscillatory plume at 200 and 1000 *bar* and a slow increase of the temperature at the wall.

Figure 4.31 shows the maximum temperature on the heater throughout the simulation with a heat flux of 200 kW/m^2 . Sixty-five, 80, and 100 *bar* have a similar growth of maximum temperature, until around 0.25 second, then there is a very sharp temperature increase leading it to pass 376.85 °C. The increase of pressure move the moment of change in a temperature gradient. For 200 and 1000 *bar*, the temperature is kept below 376.85 °C until around 2 seconds. The transition from fast growth to stabilization helps the simulation to stay under the limit.

Figure 4.32 shows the average wall temperature at the heater cylinder for all the pressures with a heat flux of 200 kW/m^2 . Ethanol at pressure 65, 80, and 100 bar did not get to the temperature stabilization, but 200 and 1000 bar got.

Figure 4.33 shows the average HTC at a heater cylinder wall for 200 kW/m^2 . Again, we see that at pressure of 65, 80, and 100 *bar* the simulations stopped before the flow reached a stabilization point, while 200 and 1000 *bar* achieved and continued the simulation until past 2 seconds.



Figure 4.29 – Temperature and y-velocity profile in the middle of the chamber for 0.25, 1, 1.5, and 2 seconds at 200 kW/m^2



Figure 4.30 – Temperature profile of the plume in different moments with a heat flux of 200 kW/m^2



Figure 4.31 – Maximum temperature at the heater cylinder wall with a heat flux of 200 kW/m^2



All simulation time interval (b) simulation time interval be

Figure 4.32 – Average temperature at the heater cylinder wall for 200 kW/m^2



Figure 4.33 – Average HTC at the heater cylinder wall with 200 kW/m^2

The most affected variable of analysis is the temperature profiles on the cylinder. Figures 4.34, and 4.35 show the profiles at 0.25 and 2 seconds with 200 kW/m^2 .

The only moment with all the pressure levels is at 0.25 seconds. At this moment, 65 *bar* has a sequence of step increases in its heater temperature, showing a degradation of the HTC right at the top. Combining this information with the properties, we see that this is a region with low specific heat at constant pressure, low density, and low thermal conductivity, similar to a vapor phase. This is an expression of the vapor-like regime of a supercritical fluid. At 80 *bar*, the fluid reached a lower temperature peak in comparison to 65 *bar*. The following flow time does not have 65, 80, and 100 *bar* due to the concerns of the EOS validity limit.



Figure 4.34 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 200 kW/m^2 at 0.25 second over the heater surface



Figure 4.35 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 200 kW/m^2 at 2 seconds over the heater surface

4.3 Correlations

The last part of the analysis is concerned with the utilization of natural convection correlation to calculate the HTC for concentric cylinders using temperature average properties and film temperature properties. The two correlations used here were presented on chapter 2, they are equations (2.37) and (2.38). The HTC used for analysis is the one just after the stabilization, a region where the flow is established but due to its transient nature continues to decrease. This means that at pressures of 65, 80, and 100 *bar* with a heat flux of 200 kW/m^2 were not possible to analyze. The fluid temperature used is 26.85 °C (300 K), and the final temperature and the wall temperature is the maximum temperature achieved at the heater at 1

second. At this moment, all the cases have established flow.

Table 4.2 shows the wall temperature used in the correlations. The bold text indicates temperatures higher than the temperature of maximum specific heat at constant pressure, the existence of pseudocritical point occurs only on 65, 80, and 100 *bar*.

P(bar)	$q \left(kW/m^2 \right)$	$T_w ^\circ C$
65.0	50.0	146.50
65.0	100.0	227.90
65.0	150.0	290.89
80.0	50.0	146.49
80.0	100.0	228.33
80.0	150.0	291.08
100.0	50.0	146.46
100.0	100.0	228.81
100.0	150.0	294.42
200.0	50.0	146.31
200.0	100.0	230.23
200.0	150.0	302.87
200.0	200.0	365.98
1000.0	50.0	136.98
1000.0	100.0	226.58
1000.0	150.0	299.98
1000.0	200.0	368.50

Table 4.2 – T_w according to the pressure and the heat flux

4.3.1 Under pseudocritical point

Table 4.3 shows the accuracy metrics, OAD, and OD in comparison to the simulated HTC for natural convection that do not reach the pseudocritical point. Equation (2.37) from Kuehn and Goldstein (1976) with integral properties got the lowest OAD, however its difference from the film temperature approach was low, under 0.05. On the other hand, equation (2.38) did not perform better with integral properties.

Table 4.3 – OAD and OD in comparison to the simulated HTC for natural convection under the pseudocritical point using equations (2.37) and (2.38) for integral properties or film temperature

Correlation and properties calculation	OAD	OD
Equation (2.37) and integral properties	0.0678	0.0656
Equation (2.38) and integral properties	0.228	-0.228
Equation (2.37) and film temperature	0.109	0.109
Equation (2.38) and film temperature	0.185	-0.185

4.3.2 Over pseudocritical point

Table 4.4 shows the accuracy metrics, OAD, and OD when the pseudocritical point were reached. The best approach was with integral properties and using equation (2.38) and integral properties. Reaching the pseudocritical point made the correlations and properties approach impact significantly on the results, the OADs were very distant from each other. However, we only have 3 points available for analysis, so it would be necessary to increase the number of heat fluxes for analysis between 100 kW/m^2 and 200 kW/m^2 in future analysis.

Table 4.4 – OAD and OD in comparison to the simulated HTC for natural convection over the pseudocritical point using equations (2.37) and (2.38) for integral properties or film temperature

Correlation and properties calculation	OAD	OD
Equation (2.37) and integral properties	0.376	0.376
Equation (2.38) and integral properties	0.0176	0.00228
Equation (2.37) and film temperature	0.166	0.166
Equation (2.38) and film temperature	0.123	-0.123

4.3.3 Summary

It is necessary a level of heat flux to reach the pseudocritical temperature for a pressure level before the stabilized transient moment. In this work, we observed only one heat flux, 150 kW/m^2 , that met this condition. The difficulty of getting this phenomena led to only 3 valid data points. When we did not have a pseudocritical point, the best approach was to use equation (2.37) with integral properties. While for simulations that reach a pseudocritical point, the combination of equation (2.38) with integral properties managed the best results. Another point is that the natural convection correlations for heat transfer coefficient were more stable using film temperature properties.

5 CONCLUSION

In this work we presented the fuel heating process at high pressure and its two possible outcomes for heat transfer, pool boiling, and natural convection, in function of pressure. If the system pressure is over the critical pressure, only natural convection will occur, but if the system pressure is under the critical one, pool boiling may also occur.

For pool boiling, we gathered data from several studies and analyzed the combination of pure component and mixture correlations for HTC calculation, and EOS. The EOS did not impact with the same capability as the correlations, also mixture correlation did not manage to influence substantially the HTC. The most prominent factor was the pure component correlation used to get the HTC for pure component equivalent on mixtures. Gorenflo and Kenning (2010) and Ribatski and Jabardo (2003) correlations had the best results. Although Ribatski and Jabardo (2003) correlation performed better on several specific conditions for fuel heating, Gorenflo and Kenning (2010) correlation had the best accuracy metrics for high pressure. The results between the other mixture correlations were similar, managing to alter only small fractions of the OAD and γ_{30} . When compared to gasoline, and blend data at low pressures, Ribatski and Jabardo (2003) correlation managed a lower OAD and a high γ_{30} .

On high-pressure fuel HTC predictions there were discrepancies between the use of either Ribatski and Jabardo (2003) or Gorenflo and Kenning (2010) correlations. Ribatski and Jabardo (2003) correlation usually underestimated in comparison to the other correlation. And as the amount of ethanol increased, the difference between the two HTC predictions got higher, it also increased with pressure and heat flux. However, only a comparison with high-pressure fuel experimental data can assure which correlation better predicts at high pressure. Despite the fact they diverged, a similar behavior was seen between them, the fast increase of HTC near the critical pressure.

Another point is the problem with the ideal heat transfer for mixtures. It is not suited for mixtures with componets at pressures higher than the pure component critical pressure. So it was not possible to evaluate beyond the lowest critical pressure from a mixture component. The change of surrogate components at high pressures might be needed to deal with low critical pressure components. However, it would only move the problem to the next low-critical pressure component. For natural convection, we did a CFD simulation of the transient supercritical flow on different conditions of pressure and heat flux with all the properties varying as a function of the temperature. Near the Widom line, the supercritical effect on the flow was seen. It caused discontinuities in temperature gradients and an increase in HTC. Beyond 150 kW/m^2 heat flux, the flow was affected by the fast increase in temperature for some pressure levels, 65 *bar*. So there is a level of heat flux that the fluid may sustain without a fast temperature increase. On pressures with a pseudocritical point, the fluid had passed the EOS temperature range with a heat flux of $200 kW/m^2$ before it could stabilize. There is a clear indicative of either turbulence or numerical instability on the simulations

Heat transfer coefficient natural convection correlations were compared with the wall average simulated heat transfer coefficient at 1 second. Using integral properties caused a higher difference between the correlations. The best combination of correlation and properties depended on if the pseudocritical temperature was achieved during the simulation. Equation 2.37 and integral properties were the best when the pseudocritical temperature was not reached, while equation 2.38 and integral properties were the best combination when the pseudocritical temperature was reached.

5.1 Future work

A comparison with experimental data is needed for both phenomena. Without this comparison, it is not possible to validate the suited correlation for pool boiling at high pressure, or to validate that the supercritical natural convection model. On the natural convection part, a turbulence model should be implemented to filter the properties peak at pseudocritical conditions and to further analyze the flow. A 3D model is required to reach a more realistic fuel heater condition, so true cylinders could be represented, showing the impact of its edges. Also, the natural convection correlations needs to be adapted to consider the heat flux instead of the wall temperature.

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A.1 Flow structure for natural convection inside a concentric cylinder

Figure A.1 – Streamlines colored by velocity magnitude and temperature scalar field for ethanol at 65 bar and with heat flux of $50 \, kW/m^2$



(a) Streamlines at t = 1s



(c) Streamlines at t = 2s



(e) Streamlines at t = 3s

Velocity 0.018

0.016

0.013

0.010

0.008

0.005

0.003

0.000 [m s^-1]



Temperature 157.355



(d) Temperature at t = 2s







(g) Streamlines at t = 4s

(h) Temperature at t = 4s

Figure A.2 – Streamlines colored by velocity magnitude and temperature scalar field for ethanol at 100 bar and with heat flux of $50 \, kW/m^2$



(a) Streamlines at t = 1s



(c) Streamlines at t = 2s



(e) Streamlines at t = 3s



(b) Temperature at t = 1s



(d) Temperature at t = 2s







Figure A.3 – Streamlines colored by velocity magnitude and temperature scalar field for ethanol at 1000 bar and with heat flux of $50 \, kW/m^2$



(a) Streamlines at t = 1s



(c) Streamlines at t = 2s



(e) Streamlines at t = 3s



(b) Temperature at t = 1s



(d) Temperature at t = 2s







Figure A.4 – Streamlines colored by velocity magnitude and temperature scalar field for ethanol at 65 bar and with heat flux of $150 \, kW/m^2$


(a) Streamlines at t = 1s



(c) Streamlines at t = 2s



(e) Streamlines at t = 3s



(b) Temperature at t = 1s



(d) Temperature at t = 2s











Figure A.6 – Streamlines colored by velocity magnitude and temperature scalar field for ethanol at 1000 bar and with heat flux of $150\,kW/m^2$



A.2 Temperature and properties profile over the heater

Figure A.7 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 50 kW/m^2 at 2 seconds over the heater surface



Figure A.8 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 50 kW/m^2 at 3 seconds over the heater surface



Figure A.9 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 100 kW/m^2 at 2 seconds over the heater surface



Figure A.10 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 100 kW/m^2 at 3 seconds over the heater surface



Figure A.11 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 200 kW/m^2 at 1 second over the heater surface



Figure A.12 – Temperature and properties - specific heat at constant pressure, dynamic viscosity, density, and thermal conductivity - profile for 200 kW/m^2 at 1.5 seconds over the heater surface