Computational fluid dynamics of advanced nuclear reactor cores and its contribution to safety analysis

Rowinski, Marcin Karol

2017

Rowinski, M. K. (2017). Computational fluid dynamics of advanced nuclear reactor cores and its contribution to safety analysis. Doctoral thesis, Nanyang Technological University, Singapore.

<http://hdl.handle.net/10356/72885>

<https://doi.org/10.32657/10356/72885>

**NANYANG
TECHNOLOGICAL
UNIVERSITY**

SINGAPORE

**COMPUTATIONAL FLUID DYNAMICS OF ADVANCED
NUCLEAR REACTOR CORES AND ITS CONTRIBUTION TO
SAFETY ANALYSIS**

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2017

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NUCLEAR REACTOR CORES AND ITS CONTRIBUTION TO
SAFETY ANALYSIS**

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A thesis submitted to the Nanyang Technological University in
partial fulfilment of the requirement for the degree of Doctor of
Philosophy

2017

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research and has not been submitted for a higher degree to any other University or Institution.

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Date

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Marcin Rowinski

Abstract

Analytical methods and Computational Fluid Dynamics (CFD) examined the safety and performance of advanced nuclear reactors. Thermal and pressure drop evaluations of an innovative annular fuel in the European lead-cooled System ELSY fast reactor were conducted. Annular fuel has superior cooling capacity, and for a square fuel lattice, the pressure drop can be lower than the reference value for standard solid fuel. Consequently, when annular fuel rods replace solid fuel rods of the same dimensions the power rating is upgraded. While the hexagonal lattice cools more effectively, the pressure drop is higher than the standard fuel assembly and incompatible with power augmentation.

Numerical investigations of supercritical flow of both carbon dioxide and water in a vertical tube under non-uniform heat flux applied at the wall demonstrated that current correlations for the Heat Transfer Coefficient (HTC) at low enthalpy values are accurate to $\pm 15\%$. At high enthalpy, only the general trend is replicated due to large property value differences near the wall and in the bulk flow. In these circumstances, the thermal conductivity, specific heat, density and viscosity are 5-8 times lower after the transition from sub- to super-critical conditions. Moreover, the efficiency of different HTC correlation models is coolant dependant, e.g. the Swenson* formula proves superior for carbon dioxide, whereas the Ornatsky model** provides better agreement with water, where a lower maximum wall temperature was obtained when a non-uniform heat flux was applied, as compared to the reference case of uniform heat flux.

For supercritical water flow inside a 2×2 fuel rod bundle, non-uniform heat flux increases wall temperature beyond the reference uniform flux. Also, wall temperature peaks occur only at the gaps between the fuel rods.

* H.S., Swenson, J.R., Carver, C.R., Karakala," Heat transfer to supercritical water in smooth-bore tubes."

**A. P. Ornatsky, L. P. Glushchenko, and E. T. Siomin, "The research of temperature conditions of small diameter parallel tubes cooled by water under supercritical pressures."

Acknowledgments

I would like to express my gratitude and appreciation to IGS for giving me the opportunity and resources for my research.

I would like to thank Professors Zhao Jiyun and Soh Yeng Chai for their valuable and constructive suggestions during the planning and development of this research work. Their willingness to give their time so generously is very much appreciated.

Besides my advisor, I would like to thank the rest of my thesis committee: Professors Timothy John White, Claude Guet and Tseng King Jet for their insightful comments and encouragement. They had posed hard questions which motivated me to widen my research from various perspectives.

I would like to show my appreciation to Dr Assel Sakanova, Dr Jan Stempien, Ms Aleksandra Tomusiak and Ms Ewa Trzaskowska for their support and motivation during hard times.

I dedicated this work to my mother Ms Krystyna Rowinska and my father Mr Marek Rowinski. Without them, I would not be where I am now.

Encouragement and support from numerous people whose names are not mentioned here are also greatly appreciated.

Publication List

Journal Articles:

- [1] M. K. Rowinski, T. J. White, J. Zhao (2015). "Innovative model of annular fuel design for lead-cooled fast reactors." *Progress in Nuclear Energy* 83: 270-282.
- [2] M. K. Rowinski, T. J. White, J. Zhao (2015). "Small and Medium sized Reactors (SMR): A review of technology." *Renewable and Sustainable Energy Reviews* 44(0): 643-656.
- [3] M. K. Rowinski, J. Zhao, T. J. White, Y. C. Soh. "Safety Analysis of Super-Critical Water Reactors - A Review". Submitted to *Progress in Nuclear Energy*
- [4] M. K. Rowinski, J. Zhao, T. J. White, Y. C. Soh. "Numerical investigation of supercritical water flow in a vertical pipe under axially non-uniform heat flux." *Progress in Nuclear Energy* 97: 11-25.
- [5] H. Cheng, J. Zhao, M. K. Rowinski (2017). "Study on two wall temperature peaks of supercritical fluid mixed convective heat transfer in circular tubes." *International Journal of Heat and Mass Transfer* 113: 257-267.

Conference Proceedings:

- [6] M. K. Rowinski, T. J. White, J. Zhao (2015). "Numerical Investigation of Supercritical Flow in a Vertical Tube under Non-Uniform Heat Flux", 23rd International Conference on Nuclear Engineering (ICONE), May 2015, *Makuhari*, Japan.
- [7] M. K. Rowinski, Y. C. Soh, T. J. White, C. C. Chieng, J. Zhao (2016). "Numerical Investigation of Supercritical Water Flow in a 2x2 Rod Bundle under Non-Uniform Heat Flux", 24th International Conference on Nuclear Engineering (ICONE), Charlotte, North Carolina, USA

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Abbreviations

4S	Super-Safe, Small and Simple reactor
ADS	Automatic Depressurization System
AECL	Atomic Energy of Canada Limited (Canada)
AFS	Auxiliary Feedwater System
AGH	AGH University of Science and Technology
AGR	Advanced Gas-cooled Reactor
AHWR	Advanced Heavy Water Reactor
ATWS	Anticipated transients without scram
BOL	Beginning of Life
BREST	Reactor designed in Russian Federation
BWR	Boiling Water Reactor
CANDU	CANada Deuterium Uranium (nuclear reactor)
CATHARE	Code for Analysis of THERmalhydraulics during an Accident of Reactor and safety Evaluation
CBR	Core Breeding Ratios
CDF	Core Damage Frequency
CEFR	Chinese Experimental Fast Reactor
CERMET	ceramic (CER) and metallic (MET) fuel
CFD	Computational Fluid Dynamics
CFD4NRS-4	4th Workshop on the CFD for Nuclear Reactor Safety
CNEA	Comisión Nacional de Energía Atómica
CNP	Chinese Nuclear Power plant
CNRS	Centre National de la Recherche Scientifique
CO ₂	Carbon dioxide
DBA	Design Basis Accident
DBA	Design Basis Accidents
DNS	Direct Numerical Simulation
DNS	Direct Numerical Simulation
DoE	Department of Energy
EC6	Enhanced CANDU-6
ECCS	Emergency Core Cooling System
ELSY	European Lead SYstem
EMP	ElectroMagnetic Pump
ENEA	National Committee for research and development of Nuclear and Alternative Energy
EOL	End of Life
FBNR	Fixed Bed Nuclear Reactor
FBR	Fast Breed Reactor

FPP	Floating Power Plant
G4M	Gen4 Module reactor
GCFR	Gas Cooled Fast Reactor
GCR	Gas Cooled Reactor
GDWP	Gravity-Driven Water Pools
GIF	Generation IV International Forum
GT-MHR	Gas Turbine – Modular Helium Reactor
HPLWR	High Performance light water reactor
HTD	Heat Transfer Deterioration
HTGR	High Temperature Gas Reactor
HTR-PM	High Temperature gas cooled Reactor – Pebble bed Module
HWR	Heavy Water Reactor
IAEA	International Atomic Energy Agency
ICS	Isolated Cooling Systems
IHX	Intermediate Heat Exchangers
IMR	Integrated Modular Reactor
iPWR	integrated Pressurized Light water Reactor
IRIS	International Reactor Innovative and Secure
KLT	Reactor designed in Russian Federation
KTH	Royal Institute of Technology
LANL	Los Alamos National Laboratory
LBE	Lead-Bismuth Eutectic
LBEFR	Lead Bismuth Eutectic Fast Reactor
LES	Large Eddy Simulation
LFR	Lead-cooled Fast Reactor
LMCR	Liquid Metal Cooled Reactors
LOCA	Loss of Coolant Accident
LOFA	Loss Of Flow Accident
LPCI	Low Pressure Injection System
LWR	Light Water Reactor
MCNP	Monte Carlo N-Particle
MCST	Maximum Cladding Surface Temperature
MDHFR	Minimum Deterioration Heat Flux Ratio
MOX	Mixed-Oxide Fuel
mPower	Reactor designed by Babcock & Wilcox
MSIV	Main Steam Isolation Valve
MSS	Moderator Safety System
Mtoe	Mega tonne equivalent
NEA	Nuclear Energy Agency
NPP	Nuclear Power Plant
NRG	Previously, Energy Research Centre of the Netherlands (ECN)
NuScale	Reactor designed in Oregon State University
PBMR	Pebble Bed Modular Reactor

PCCS	Passive Containment Cooling System
PFBR	Prototype Fast Breed Reactor
PHRS	Passive Residual Heat Removal System
PHWR	Pressurized Heavy Water Reactor
PIE	Postulated Initial Event
PIE	Postulated Initial Event
PRISM	Power Reactor Inherently Safe Module
PSA	Probabilistic Safety Analysis
PWR	Pressurized Water Reactor
RANS	Reynolds-Averaged Navier–Stokes
RBMK	High Power Channel-type Reactor
REFPROP	NIST Reference Fluid Thermodynamic and Transport Properties Database
RELAP	Reactor Excursion and Leak Analysis Program
RFA	Robust Fuel Assemblies
RPV	Reactor Pressure Vessel
RSM	Reynolds Stress Model
SACoS	Subchannel Analysis Code of SCWR
SCFBR-D	Supercritical Light Water cooled Fast Breeder Reactor
SCFR-D	Supercritical Light Water cooled Fast Converter Reactor
SCLWR	Supercritical Light Water cooled Reactor
SCRIPT	Supercritical water cooled IN-PILE Test
SCWR	SuperCritical Water-cooled Reactor
SCWR-FQT	Supercritical Water Reactor – Fuel Qualification Test
SFR	Sodium Fast Reactor
SG	Steam Generator
SLCS	Standby Liquid Control System
SMART	System-integrated Modular Advanced Reactor
SMR	Small Modular Reactor or Small and Medium Sized Reactor
SPHINX	Supercritical Pressure Heat transfer Investigation for NeXt generation
SSCWR	Simplified SuperCritical Water-cooled Reactor
SSR	SuperSafe Reactor
Super LWR	Supercritical Light Water cooled Reactor
SVBR	Reactor designed in Russian Federation
TACOS	Transient Analysis Code Of SCWR
TMI	Three Mile Island
TRISO	(TRIstructural-ISOtropic)
UNITHERM	Reactor designed by Research and Development Institute of Power Engineering
VVER	Water-Water Energetic Reactor
YSZ	Yttria Stabilized Zirconia

Symbols

μ	Dynamic viscosity	[Pa s]
A	Area	[m ²]
c_p	isobaric specific heat	[J/kg K]
D	Element diameter	[m]
D	Diffusion coefficient	[cm]
D_H	Hydraulic diameter	[m]
F_H	Axial peaking factor	-
F_R	Radial peaking factor	-
g	Gap between elements	[m]
h	Heat transfer coefficient	[W/m ² K]
J	Diffusion flux	[1/cm s]
k	Thermal conductivity	[W/m K]
L	Specific length	[m]
m	Mass flow rate	[kg/s]
N	Number	-
Nu	Nusselt number	$\left(\frac{hD}{k} \right)$
P	Power	[W]
p	Pitch between elements	[m]
Pe	Peclet number	$\left(\frac{Lv}{D} \right)$
Pr	Prandtl number	$\left(\frac{\mu c_p}{k} \right)$
q	Heat	[W]
q''	Heat flux	[W/m ²]
q'''	Volumetric heat flux	[W/m ³]
R	Radius	[m]
Re	Reynolds number	$\left(\frac{mD}{\mu} \right)$
T	Temperature	[K] or [°C]

v	Velocity	[m/s]
V	Volume	[m ³]
W	Wetted perimeter	[m]
w	recoverable energy	[J or MeV]
α	Thermal diffusivity	[m ² /s]
β	Ratio between new and default fuel volume	[%]
γ	Ratio of heat transfer surface to total heat transfer surface	-
δ	Ratio between coolant and fuel volume	-
Δp	Pressure drop	[Pa]
ρ	Density	[kg/m ³]
σ	Microscopic cross section	[cm ²]
Σ	Macroscopic cross section	[1/cm]
ν	average number of neutrons produced per fission	-
ν	viscosity	[m ² /s]
ϕ	Neutron flux	[1/cm ² s]

Superscripts

avg	Average
max	Maximum

Subscripts

as	Assemble
b	Bulk
c	Cladding
cr	Critical
e	Element
el	Electrical
f	Fuel
g	Gas gap
i	Inner
in	Inlet
o	Outer
Out	Outlet

Pb	Lead
pc	Pseudo-Critical
ref	Reference
th	Thermal
w	Wall

Chapter 1

Introduction*

The key objective of this thesis is to use thermal-hydraulics and computational fluid dynamics to provide improved understanding and enhance the safety of nuclear fuel elements. This chapter explains the purpose and motivation behind the research, and consists of five subsections, beginning with the problem statement and need for safe and clean nuclear energy. This is followed by a brief description of various reactor types. Subsequently, the research objectives including the development and evaluation of annular fuel for lead-cooled fast reactors and the evaluation of supercritical flow are examined. A brief overview of the thesis, including a compilation of the projects completed and a description of the content of each chapter are then provided. Finally, a summary of the outcomes are presented.

*This section published substantially as reference: Rowinski et al. (2015). "Small and Medium sized Reactors (SMR): A review of technology." Renewable and Sustainable Energy Reviews **44**(0): 643-656

1.1 Problem Statement

The modern world is energy intensive and per capita consumption is growing. In 2013, global energy generation was 13,541 Mtoe (Mega tonne equivalent) from primary sources, with the greatest share from oil and coal [1]. Fig 1-1 presents the changing energy supply mix and shows total capacity is now more than 350% higher than in 1965. While every energy source has increased, including polluting fossil fuels, particularly after the year 2000, renewables are growing more slowly due to their presently higher cost (e.g. photovoltaic) or limited availability (e.g. hydro).

Coal, oil and gas produce 67.4% of electricity globally [1], with less than one-third of electricity produced from “green” sources (Fig. 1-2). The dominant “green” technology is hydropower plants with total electricity production equal to nuclear and others (renewables) combined. Pioro et al. [2-4] state that gas combined-cycle power plants are the most efficient for power generation (62% efficiency), followed by supercritical pressure coal-fired thermal power plants (55% efficiency). Current Nuclear Power Plants (NPPs) have efficiencies below 50%, with the dominant Light Water Reactors operating up to 35%. Generation IV NPPs are designed for efficiencies of between 45-50%.

Fig. 1-1 World primary energy supply in Mtoe [5]

Fig. 1-2 Electricity generation by fuel [1]

The emission of carbon dioxide (CO_2) compared has grown in tandem with electricity production, and increased rapidly with higher coal consumption, and is now 170% higher than in 1985 (Fig. 1-1 and Fig. 1-3.). This is of concern as CO_2 contributes to the greenhouse effect that accelerates climate change, and it is urgent to mitigate these effects through the adoption of environmentally benign technologies. A promising alternative is nuclear power that emits minimal gases, but creates radioactive waste that can be stored in special facilities. While there have been three severe accidents, nuclear energy offers electricity generation independent of weather and less susceptible to economic shocks.

Fig. 1-3 World electricity generation and carbon dioxide emission [5]

Nuclear energy has been in production for over 60 years. According to the International Atomic Energy Agency (IAEA) [6], there are 438 Nuclear Power Plants (NPPs) with a total capacity of 376.2 GW(e) in operation and 70 reactors are under construction globally [6]. As most reactors (81.5%) are light water moderated and cooled, this technology has priority in research and license processing of new designs. These reactors use light water under subcritical conditions ($T_{cr} = 374^{\circ}\text{C}$, $p_{cr} = 22.115\text{MPa}$) that limit the maximum efficiency to around 35%. The SuperCritical Water-cooled Reactors (SCWRs) and other advanced reactors have projected efficiencies of 48% that is comparable to conventional thermal power plants.

In 2001, the “nuclear renaissance” or “second nuclear era” [7] commenced with nuclear power plants planned and construction started in countries that had withdrawn from nuclear energy [8], including the first nuclear power plant in the USA since the Chernobyl accident in 1986 [9]. The best demonstration of the second nuclear era is in China, with 36 nuclear reactors in operation and 21 under construction as of May 2017 [10]. The most recent nuclear accident was on 11th March 2011 in Fukushima, Japan. A huge earthquake followed by a tsunami caused flooding of the auxiliary diesel cooling system and loss of vessel containment resulting in a hydrogen explosion and radioactive leakage [11]. In the aftermath, Japan reorganized the national energy mix, and currently, all NPPs are suspended or shut down for maintenance. In mid-August 2015, Sendai 1 was the first reactor restarted after the Fukushima accident with 2 units in operation and 23 under review [12]. Post Fukushima, some countries most notably Germany, shut down all NPPs [13], while France is decreasing its reliance nuclear energy. Therefore, the Fukushima accident was instructive, rather than a critical blow to the industry. Only a few countries withdrew from nuclear energy, with most retaining the option as part of their energy policy.

To date, the majority of commercial Nuclear Power Plants (NPPs) are large installations ($> 1\text{GW}_{el}$), but for remote and inaccessible areas including Alaska and the Russian tundra, there is a case for small units to supply electricity and potable water [1]. Recently, substantial research effort has been directed towards the development of Small Modular Reactors (SMRs) of capacity less than 700MW_e . China, despite investing in large nuclear power plants [2], is also developing small reactors [3]. Other countries support licensing programs of small modular reactor designs, including the US

Department of Energy (DoE) that anticipates a 5-year Licensing Technical Support Program worth \$452M for light water reactor designs and another program for Generation IV designs [4]. Separately, technologies to convert Generation III/III+ to safer and more reliable Generation IV nuclear reactors are under development. Recently, nuclear power reactors for marine applications such as propulsion or as floating power plants (FPP) are receiving greater attention [14].

1.2 Reactor Designs

According to the Generation IV International Forum [15] reactors can be grouped into four generations:

- (i) *Generation I (1950 – 1970)*: first prototypes of numerous different designs and approaches, including water and gas cooled reactors;
- (ii) *Generation II (1970 – 1995)*: commercial nuclear power plants, Light Water Reactors (LWRs) and Heavy Water Reactors (HWRs), and the emphasis is on power generation;
- (iii) *Generation III/III+ (1995 – 2030)*: improvement of Generation II reactors;
- (iv) *Generation IV (2030)*: new reactor designs that are more efficient than previous generations.

Contemporary commercial nuclear power plants are Generation III/III+, with the remaining Generation II plants to be decommissioned in the near future. Currently, no commercial Generation IV nuclear power plant is in operation. The Sodium Cooled Reactor Phénix, in France, was shut down in 2009 after obtaining criticality in 1973 [16]. Large reactors and Small Modular Reactors (SMRs) should incorporate [17, 18]:

- (i) inherent and passive safety engineering to assure security during normal operation and accidents;
- (ii) proliferation resistance;
- (iii) economic competitiveness with other power generation technologies;
- (iv) a probability of severe accident that is below 10^{-5} accident per year; and
- (v) ease of operation and maintenance.

SMRs should also be transportable from the factory to the field. Fig. 1-4 shows the classification of SMRs according to generation, neutron spectrum and coolant.

Fig. 1-4 SMR classification

Table 1-1 summarizes the characteristics of SMR generation IV nuclear reactors and their estimated performance. Compared to larger units, the small power density of SMRs permits the deployment of passive cooling systems. This also eliminates large volume Loss of Coolant Accidents (LOCA) triggered by small pipe diameters exiting the vessel [19]. However, the small power density yields a lower efficiency in comparison to the larger units; especially in the case of water reactors.

The acronym SMR can describe a small modular reactor [7] that is factory built and assembled then shipped to site. However, according to the International Atomic Energy Agency (IAEA), SMR also stands for Small and Medium Sized Reactor [20-22]. Small reactors are those below 300MW_e and medium are those between 300-700MW_e that are suitable for smaller power grids or remote locations where a connection to existing power grids would not be economically justified. For example, OKBM Afrikantov designed a floating nuclear power plant [14].

High temperature reactors provide quality steam suitable for industrial applications such as desalination [23], hydrogen gas production [24], or even combined with off-shore wind farms [25]. Most small modular reactor fuels show higher burn-up to extend the time between refueling [26, 27]. Some are planned to operate without refueling for 30

years [28] and could work their whole lifetime without the need to shut down for refueling.

Table 1-1 Summary of SMR technology [18-20, 29-39][40-50]

Technology	LWR	HWR	SFR	LFR/LBEFR	GCR
Efficiency (%)	25-35	30-35	30-40	35-45	40-50 (theoretically)
Thermodynamic Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle or Brayton Cycle
Design Life (y)	25-60	40-100	30-40	35-43	40-60
Fuel Type	UO ₂ , TRISO or CERMET	(Th-233U)O ₂ , (Th-Pu)O ₂ or UO ₂	U-Pu-Zr alloy or (Pu-U)O ₂	PuN-UN, UN, UO ₂	TRISO UO ₂
Enrichment (%)	1.8-19.75	0.711 - 4	16.6-19.75	16.4-19.75	8.5-weapon grade plutonium
Refuelling Period (months)	14-240	24 - online	6 - end of design life	84-120	10 - online
Reactor Vessel Circulation	Forced or Natural	Forced	Forced	Forced or Natural	Forced

Small modular reactors have inherent and passive safety systems as part of a “defense in depth” approach [21, 32, 51, 52]. Usually core heat is removed by natural convection inside the Reactor Pressure Vessel (RPV) [53] so that during a malfunction or severe accident, the reactor will shut down without operator intervention. This thesis explores the passive safety and efficiency of SMR designs using two approaches:

- (i) ***Investigation of innovative annular fuel assemblies in Lead-cooled Fast Reactors.*** In this section, comprehensive analysis of nuclear fuel element thermohydraulics underpins innovative fuel designs to improve performance and safety margins that exploits the superior cooling capacity of Lead-cooled Fast Reactors (LFRs). These insights in fuel bundle performance provide a useful comparative reference for Generation IV reactors.

- (ii) ***Modelling of thermal response in supercritical conditions.*** Computational Fluid Dynamics (CFD) modelling of fuel rod thermal responses in advanced nuclear reactors are crucial in SuperCritical Water-cooled Reactors (SCWRs). These approaches are required to understand the trade-off of performance against safety.

The LFRs and SCWRs were jointly studied because both are Generation IV reactors sharing common features. The investigations focused on Generation IV reactor safety examine the impact of thermodynamics and fluid mechanics. Here, the main focus is on the thermohydraulics and CFD, and although neutronics is of critical importance, this was not considered within the current scope of work. The inclusion of neutronics would be a natural extension of the current investigation.

1.3 Research Objectives

The motivation of this research is to examine those features of advanced Generation IV nuclear reactor designs that contribute to safe operation. The objectives were:

1. *To develop a thermodynamics model for the standard fuel design of a Lead-cooled Fast Reactor (LFR):*

The model will estimate parameters such as pressure drop through the fuel assembly, and the temperature distribution in average and “hot” fuel rods. The estimation considers the fuel rods density, fuel rod gap, and inner and outer cladding diameters. The modelling will compare solid rod and annular tube fuel concepts.

2. *Model optimization according to technical criteria and limits:*

The model takes into account technical criteria and limits for LFR and construction materials. The most promising designs will be selected for further analysis, taking into consideration multiple aspects of the fuel assembly.

3. *Design of CFD simulation of vertical supercritical flow of water and carbon dioxide under various heat flux:*

Numerical investigations of supercritical flow in a vertical pipe include various applied heat fluxes at the wall to evaluate if heat transfer correlations can predict the Heat Transfer Deterioration (HTD) phenomenon accurately. The CFD simulations will also consider how non-uniform heat flux influences the thermal response.

4. Design of CFD simulation of nuclear fuel bundle:

Here, a calculation domain of 2×2 fuel rod bundles based on the literature reports will be designed. After validation, the simulations were applied to a non-uniform heat flux, especially the thermal response at the fuel rod walls as a function of the angle position.

1.4 Overview

The thesis is organized as follows:

Chapter 2 contains a literature review of Small Modular Reactors (SMRs). It provides a historical perspective, nuclear reactions, fuel cycles, reactor technologies including strengths and limitations, safety features, proliferation impacts, and computational tools.

Chapter 3 presents the methodology used during the research based on fluid dynamics and thermodynamics. The thermodynamic principles used during analytical analyses are described and an explanation of computational fluid dynamics simulations is included.

Chapter 4 describes the innovative annular fuel design, its concept and possible application in a Lead-cooled Fast Reactor. This chapter provides information concerning the design process and research results, especially the thermal response and pressure drop along the fuel channel.

Chapter 5 presents a safety analysis of SuperCritical Water-cooled Reactors, through a comprehensive literature review of common SCWR design concepts. It presents the development status of the various designs.

Chapter 6 presents the numerical investigation of a supercritical flow of carbon dioxide in a vertical tube, focusing on thermal properties of the flow and thermal response under a non-uniform heat flux. The results are compared to analytical solutions to evaluate if the currently used heat transfer formulae are applicable under supercritical flow.

Chapter 7, similar to Chapter 5, investigates the supercritical flow in a vertical flow, however, in this case the working medium is water. Again, the thermal response and heat transfer coefficients are considered.

Chapter 8 presents the numerical investigation of a 2x2 fuel rod bundle, especially the wall thermal response under various applied heat flux. The main interest is in the wall temperature at different angles of the heated rod.

Chapter 9 concludes the thesis and gives several recommendations and an outlook for possible future work.

1.5 Outcomes

The research outcomes of this thesis are as follows:

1. An innovative design of an annular fuel lattice for a lead-cooled fast reactor was modelled. This geometry delivered superior heat removal properties compared to standard solid nuclear fuel rods and offered higher safety margins.
2. CFD calculations accurately predicted the thermal response of supercritical flow. By comparing the heat transfer correlations it was found that the Bishop's and Ornaty's formulae are the most accurate predictors of supercritical water and carbon dioxide behavior. Moreover, these algorithms can forecast heat transfer deterioration phenomenon at the correct geometric position.
3. The supercritical flow in a rod bundle is characterized by the non-symmetrical thermal response at the angle position of the fuel rods.

Chapter 2

Literature Review*

A Nuclear Power Plant (NPP), as does any thermal power station, uses heat to generate high temperature steam to run a turbo generator and produce electricity. In an NPP, a nuclear reactor takes the role of a boiler by hosting the exothermic atom fission reaction. This chapter reviews 25 Small and Medium sized Reactor designs currently under development, licensed or in operation, with a particular focus on Lead-cooled Fast Reactors (LFRs) and SuperCritical Water-cooled Reactors (SCWRs). In this technology assessment, safety features and the ability to mitigate proliferation are particularly considered. In order to show common research trends and highlight key features of particular designs, the reactors were classified according to design and cooling medium. The main requirement for new reactor designs is to secure inherent and passive safety features, and different ways to achieve this outcome are compared. Furthermore, the use of innovative reactor designs can mitigate proliferation concerns to an acceptable level. The common research elements among all designs, especially in fuel cycle evaluation and optimization are identified.

*This section published substantially as reference: Rowinski et al. (2015). "Small and Medium sized Reactors (SMR): A review of technology." Renewable and Sustainable Energy Reviews **44**(0): 643-656

2.1 Introduction

Economic development and population growth demand a growing secure energy supply, especially electrical energy. One of the most reliable and sustainable power technologies is nuclear power whose output is independent of weather (a problem for renewables) and economic conditions (when commodity prices fluctuate). The majority of commercial Nuclear Power Plants (NPPs) have high electrical power output ($> 1 \text{ GW}_{\text{el}}$), yet the trend in power generation is shifting to smaller units, in order to supply electricity to remote locations, or on ships, to create distributed energy systems. Recently, substantial research has focused on designing and demonstrating small nuclear reactors. The Small and Medium-sized Reactors (SMRs) and Generation IV reactors present opportunities to create an energy system that is more flexible, and thus suitable, for current energy strategies.

2.2 Historical Background

Nuclear power can be traced to the discoveries of by Otto Hahn and Fritz Strassmann who in 1938 observed the fission of uranium-235 (^{235}U) [54]. The nuclear era began on 2nd December 1942, when Enrico Fermi initiated the first critical, self-sustaining, chain reaction in Chicago Pile-1. It was a stockpile of pure natural uranium serving as the fuel and graphite was used as a moderator with control rods of cadmium, indium, and silver. There was neither cooling, nor radiation shielding as Fermi assumed these were unnecessary [55]. The first nuclear reactors were for military purposes, but in time, reactors were introduced commercially as reliable and low CO_2 emission sources of electricity. The first NPP, Obninsk, was built in the former Soviet Union in 1954 [56], followed in 1956 by Calder Hall 1 in the United Kingdom [57, 58]. The introduction of commercial NPPs created a “boom” for nuclear energy. Reactors became ever more powerful, presently reaching $1650 \text{ MW}_{\text{el}}$. The core volume decreased due to water cooling and enriched fuel which provided a higher power density. This nuclear expansion ended with the Chernobyl accident, after which the growth of nuclear power slowed considerably and ceased in some countries [59-61]. Before the accident, it was generally forecast that the number of NPPs would increase with improved safety and availability [62]. However, Chernobyl proved more influential than the first nuclear incident in 1979 at Three Miles Island, USA, where the reactor core melted. Nonetheless, lessons were learned and new safety standards introduced [63-65].

2.3 Nuclear Reactions

A key reaction in thermal spectrum nuclear reactors is **elastic scattering**. In this case, a neutron impacts a nucleus in the ground state then deflects, leaving the nuclear structure unchanged. The neutron changes direction and velocity, and the nucleus recoils with energy preserved as the neutron slows. This reaction may occur between a neutron and any nucleus. For example, the reaction between a neutron (n) and hydrogen (H) is:

In thermal reactors, neutrons slow to a velocity specific for ambient temperature, i.e. 20°C. Of specific interest are collisions with light nuclei where the smaller mass difference between the particles means a higher kinetic energy is exchanged. This is the basic principle of moderation.

In **inelastic scattering**, the neutron is striking a nucleus and leaves it in an excited state. The nucleus then decays, usually quickly, back to the ground state by emission of gamma photon(s). Such reactions are endothermic and not desirable in the reactor. An example of the inelastic scattering of a neutron and uranium-238 (${}^{238}\text{U}$) is:

The asterisk indicates the excited state of the nucleus. This reaction can only occur if the neutron energy is higher than that of the lowest excited energy of a struck nucleus. Because of energy conservation, the total kinetic energy is equal to the sum of the kinetic energies of the neutron, ${}^{238}\text{U}$ and excitation energy. The heavier the nucleus, the lower is the energy needed to excite a nucleus.

Neutron capture is one of the exothermic neutron absorption reactions. Here, the neutron is captured by the nucleus and gamma photon is emitted as a result. The reaction consists of two stages, the first neutron is captured by the nucleus and the heavier isotope is created in the excited state, then the nucleus decays to ground state. An example of such reaction is:

This reaction may occur for almost any nucleus, and for heavy particles can lead to fissile elements for nuclear fuel. The example above shows the beginning of the production of plutonium-239 (${}^{239}\text{Pu}$), through decay to neptunium-239 (${}^{239}\text{Np}$) and then decay to ${}^{239}\text{Pu}$.

Neutron producing reactions generate an additional neutron(s) extracted from a nucleus. This reaction is especially important in reactors containing heavy water or beryllium as neutrons are easily endothermic ejected:

As is well known, the exothermic **nuclear fission** reaction becomes self-sustainable because 2 or 3 neutrons promulgate a chain reaction such as:

Such reactions can occur for almost any nucleus but are exothermic only for nuclides heavier than iron-56 (${}^{56}\text{Fe}$). Moreover, highly energetic neutrons are required and, thus only a few nuclei can undergo fission. A range of fission products are produced with the preservation of sums of atomic numbers and with mass numbers of 92 and 236, respectively.

The **microscopic cross section** $\sigma_f^{(i)}(E)$ is the probability of a given reaction occurring dependent on the neutron energy E . The cross section unit is the barn that ranges from 10^{-24}cm^2 or 10^{-28}m^2 . The total cross section is the sum of coherent and incoherent scattering for the nucleus. The **Macroscopic cross section** is the probability per unit length (cm^{-1}) traveled that a neutron will undergo a reaction with a nucleus. **Fissile material** contains nuclei that undergoes fission through interaction with low energy neutrons and is suitable as a nuclear fuel. The only fissile material that occurs in nature is ${}^{235}\text{U}$; with all other nuclides in nuclear reactors, i.e. ${}^{233}\text{U}$, ${}^{239}\text{Pu}$, and ${}^{241}\text{Pu}$, and breeder reactors can be designed where the rate of production exceeds the rate of utilization. **Fertile materials** such as ${}^{238}\text{U}$ and ${}^{232}\text{Th}$ can be transformed into a fissile material after absorption of a neutron (see Fig. 2-1) to produce a

nuclear fuel over a period of days to months. Table 2-1 lists the most common fertile materials and their transmuted fissile products.

Fig. 2-1 Examples of transformation of fertile materials into fissile materials

Table 2-1 List of fertile materials and their fissile products

Fertile Material	Fissile Material
Thorium-232	Uranium-233
Uranium-234	Uranium-235
Uranium-238	Plutonium-239
Plutonium-238	Plutonium-239
Plutonium-240	Plutonium-241

2.4 Fuel Cycles

Uranium and thorium fuel cycles are the sum of processing steps involved from fuel fabrication from an ore to its disposal after use [39, 66]. In an open cycle, spent fuel is not reused and requires disposal. A closed fuel cycle, on the other hand, incorporates reprocessing where uranium, plutonium or other actinides are extracted from the spent fuel for re-fabrication as a fuel [67]. Therefore, uranium and thorium resources are depleted more slowly to secure fuel supplies for an extended period of time. The most mature mixed-oxide fuels (MOX) contain uranium and plutonium recovered from nuclear warheads. This cycle has been completely developed in France [68].

2.5 Heavy Water Reactors

Heavy Water Reactors (HWRs) are the second most common reactor design after LWR with a world-wide installation of nearly 50 units, especially in Canada and India (Table 2-2). A key advantage of this technology is simplified refueling. Because the moderator is heavy water, the fuel can be natural or slightly enriched uranium contained in calandria around the fuel assemblies. The coolant can heavy or light water depending on the design.

Table 2-2 Summary of Heavy Water Reactors [37-39]

Design Name	AHWR300-LEU	EC6	PHWR-220
Origin Country	India	Canada	India
Electric Power (MW _e)	304	740	236
Efficiency (%)	33	35	31
Coolant	Light Water	Heavy Water	Heavy Water
Reactor Pressure (MPa)	7	10.09	8.5
Core Outlet Temperature (°C)	285	310	293
Design Life (years)	100	60	40
Fuel Type	(Th-233U)O ₂ , (Th-Pu)O ₂	UO ₂	UO ₂
Enrichment (%)	3-3.75% 233U, 2.5-4% Pu	natural	natural
Refuelling Period (months)	online	online	24

2.6 Light Water Reactors

Light Water Reactors (LWRs) are widely deployed with 357 LWRs out of 437 reactors in operation, including 273 Pressurized Water Reactors (PWR). This long operational experience with PWR expedites licensing and is the only LWR reactor type under consideration in every country that pursues SMRs (Argentina, Brazil, China, France, Republic of Korea, Russian Federation and the United States of America), where the inherent passive safety of is preferred. Table 2-3 summarizes SMRs using light water as a coolant and moderator. PWR use dual coolant loops. The primary coolant system, which removes energy produced by the fission reaction in the core, is under very high pressure (ca. 15 MPa) in order to liquidly water at high temperature. Energy is transferred to the secondary coolant system where water is boiled at high pressure (ca. 7 MPa) to produce high-quality steam. This heat exchanger is a steam generator (SG) used to run the turbine to produce electricity.

Table 2-3 Summary of Pressurized Water Reactors [1, 2, 22-24, 27-32]

Design Name	CAREM	FBNR	CNP-300	FLEXBLUE	IMR	SMART	KLT40-S	UNITHERM	IRIS	mPower	NuScale	Westinghouse SMR
Origin Country	Argentina	Brazil	China	France	Japan	Korea	Russia	Russia	International	USA	USA	USA
Electric Power (MW _e)	25	40	325	160	350	100	35	6.5	335	150	45	225
Efficiency (%)	25		33	25	35	30	23	21	33	30	28	28
Thermodynamic Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle	Steam Rankine Cycle
Reactor Pressure (MPa)	12.25	16	15.2	15.5	15.51	15	12.7	16.5	15.5	14.1	8.72	15.5
Core Outlet Temperature (°C)	326	326	302	310	345	323	316	325	330	320	329	310
Design Life (years)	60	N/A	40	60	60	60	40	25	60	60	60	60
Fuel Type	UO ₂	TRISO or CERMET	UO ₂	UO ₂	UO ₂	UO ₂	UO ₂	CERMET	UO ₂ /MOX	UO ₂	UO ₂	UO ₂
Enrichment (%)	1.8, 3.4	5 - 9	2.4-3	5	4.8	4.8	<20	19.75	4.95	<5	4.95	<5
Refuelling Period (months)	14	36 - 84	18	36	26	36	28	240	48	48	24	24
Circulation in RPV	Natural	Forced	Forced	Forced	Forced	Forced	Forced	Natural	Forced	Forced	Natural	Forced

2.7 SuperCritical Water-cooled Reactors

SuperCritical Water-cooled Reactors (SCWR) use steam above critical conditions (over 22.064 MPa and 374°C) to run a turbine and combines a high-efficiency thermal power plant and a nuclear power source. The concept integrates elements of the Boiling Water Reactor (BWR) with the Light Water Reactor (LWR) design, i.e. light water coolant flows inside pressurized tubes and exits the core at 625°C from 25 to 26 MPa that is above the critical point. As water properties vary across the sub- to supercritical boundary, working above the critical point avoids fluid phase changes and the properties change continuously [69].

Only one SMR design of the SCWR type is undergoing development. The SuperSafe Reactor (SSR) is the scaled version of the Canadian Deuterium Uranium CANDU-SCWR proposed by Atomic Energy of Canada Limited AECL [70]. The power output is estimated to be 300MW_{el} with an efficiency of ca. 45%, which is much higher than conventional water reactor efficiency of up to 35%. The CANDU design ensures that heavy water is stored in the calandria at near-ambient conditions, ensuring proper moderation of neutrons and eliminating control rod rejection accidents.

SCWR is the only reactor technology not yet in operation, but work is in progress to adjust current safety codes for supercritical fluids through implementing appropriate heat transfer coefficient relationships. Modelling supercritical flow minimizes the need to build expensive test loops [71]. Other challenges include finding universal heat transfer coefficient correlations for any flow parameters [72] and the selection of An investigation of alternative fuels i.e. UC and UO₂-BeO [73].

This thesis is concerned with the modelling of supercritical flow in SCWRs in bare vertical tubes and the thermal response.

2.8 Liquid Metal Cooled Reactors

The Liquid Metal Cooled Reactor (LMCR) is a fast reactor concept where liquid metal is the coolant, and a moderator is unnecessary as fast spectrum of neutrons are used. The two designs are the loop and pool concepts. The first approach, found in Sodium-cooled Fast Reactors (SFRs), uses two loops containing liquid metal with two heat exchanger systems

producing steam. The second approach, places heat exchangers/steam generators inside the reactor and is common in Lead-cooled Fast Reactors (LFRs). The efficiency of large FBRs exceeds conventional water reactors as the reactor vessel sustains higher temperatures (Table 2-4).

While LMCRs have proven less popular than other technologies, due to risks associated with the high melting temperature in LFRs, or violent exothermic reactions in contact with water in SFRs, naval propulsion systems have operated without major accidents [74]. LFRs are only used in shipping, whereas the SFRs were used to produce electricity [75]. The first sodium reactor named BN-350 went online in 1973 in Aktau, Kazakhstan [76], and later the same year in Marcoule, France, when the Phénix reactor was connected to the grid [77].

Fast-breeder metal cooled reactors (FMCR) produce nuclear fuel with a breeding ratio greater than unity. Moreover, transmutation of nuclear waste from conventional reactors is possible. Therefore, the fuel cycle is closed, nuclear waste will be less problematic and finite uranium reserves are extended. The European Lead System (ELSY) pool type reactor is a pure lead fast spectrum reactor of 600MW_e power capacity being developed under the Sixth EURATOM Framework Programme by ENEA (National Committee for research and development of Nuclear and Alternative Energy), NRG (Previously, Energy Research Centre of the Netherlands (ECN)), CNRS (Centre National de la Recherche Scientifique) and universities such as KTH (Royal Institute of Technology), Sweden and AGH (AGH University of Science and Technology), Poland [43].

The design consists of eight steam generators inside the reactor vessel with integrated pumps to force circulation. For heat removal, natural circulation inside the reactor vessel is sufficient. The proposed fuel is a MOX nitride fuel with three Pu enrichment zones to flatten the outlet coolant temperature. For two fuel lattice designs, i.e. open square and closed hexagonal [78-80], the thermal hydraulics, core design, corrosive and erosive resistive materials together with feasibility and economic estimations are being investigated.

For this thesis work, the European Lead-cooled SYstem (ELSY) was chosen for further research with respect to thermal hydraulics of the fuel.

Table 2-4 Summary of Liquid Metal Cooled Reactors [36-43]

Design Name	4S	BREST-OD-30	CEFR	G4M (Hyperion)	PFBR-500	PRISM	SVBR-100	ELSY
Origin Country	Japan	Russia	China	USA	India	USA	Russia	European Union
Electric Power (MW _{el})	10	300	20	25	500	311	101	600
Efficiency (%)	33	43	30	35	40	37	39	42
Coolant	Sodium	Lead	Sodium	Lead-Bismuth Eutectic	Sodium	Sodium	Lead-Bismuth Eutectic	Lead
Reactor Pressure (MPa)	Near ambient	Near ambient	Near ambient	Near ambient	Near ambient	Near ambient	6.7	Near ambient
Core Outlet Temperature (°C)	510	540	530	500	547	485	500	480
Design Life (years)	30	60	30	10	40	N/A	60	60
Fuel Type	U-Pu-Zr alloy	PuN-UN	(Pu-U)O ₂ - MOX	UN	(Pu-U)O ₂ - MOX	U-Pu-Zr alloy	UO ₂	PuN-UN
Enrichment (%)	19	N/A	16.6	19.75	NA (Two zones)	N/A	16.4	14.54/17.63/20.61 Pu
Refuelling Period (months)	No refuelling	N/A	N/A	120	6	18	84-96	5 (residence time 20 months)
Circulation in RPV	Forced	Forced	Forced	Forced	Forced	Forced	Natural	Forced

2.9 Gas Cooled Reactors

Gas Cooled Reactors use helium or carbon dioxide as a coolant where the moderator is usually graphite blocks (Table 2-5). This is the oldest approach in nuclear reactor history but not used commonly in energy production due to the poor power density. A unique fuel is the tristructural-isotropic TRISO type where a small uranium or plutonium core is coated with graphite and silica. The reactor can incorporate either an indirect Rankine steam cycle or direct Brayton cycle achieving up to 50% efficiency at around 1000°C.

Table 2-5 Summary of Gas Cooled Reactors [48-50]

Design Name	GT-MHR	HTR-PM	PBMR
Country of Origin	USA	China	South Africa
Electric Power (MW_{el})	150	200	164
Efficiency (%)	42	40	41
Thermodynamic Cycle	Brayton Cycle	Steam Rankine Cycle	Brayton Cycle
Coolant	Helium	Helium	Helium
Reactor Pressure (MPa)	6.39	7	9
Core Outlet Temperature (°C)	750	750	900
Design Life (years)	60	40	60
Fuel Type	TRISO UO ₂	TRISO UO ₂	TRISO UO ₂
Enrichment (%)	15.5	8.5	9.6
Refuelling Period (months)	18	online	10

2.10 Safety Features

New generation reactor designs must satisfy high safety requirements in order to pass increasingly demanding licensing procedures due to accidents such as Three Mile Island (TMI), Chernobyl and Fukushima that take into account new accident scenarios. For example, Fukushima revealed that active decay heat removal systems are insufficient if their functionality is crucial in the beginning of an accident. Therefore, contemporary safety systems must secure heat removal from the RPV for the first few hours during the

shutdown without active actuation. The operability of the safety systems should be independent of environmental conditions such as flood or earthquake.

The products of the fission reaction must not spread to the environment during both operational and accidental conditions, and the design must consist of multiple robust barriers. Another requirement is negative temperature and void reactivity coefficients to assure self-stability of the core.

2.10.1 Heavy Water Reactors

Safety features are reactor specific. The Indian AHWR is the state-of-the-art among heavy water reactors and the only one with independent passive safety features. Natural circulation removes heat during operation and shutdown, even during critical pump failure. The Emergency Core Cooling System (ECCS) consists of borated water accumulators together with Gravity-Driven Water Pools (GDWP) connected to four independent loops that can secure the core in a LOCA scenario for at least 72 hours. The calandria contains heavy water at near-ambient pressure to reduce the possibility of leakage secured with a moderator passive cooling system to minimize tritium release to should the pressure increase due to a temperature rise.

2.10.2 Light Water Reactors

The integrated design is the most common light water PWRs with pressurizer and SGs inside the RPV. As the primary coolant system is inside the RPV, the possibility of LOCA are reduced because natural circulation in the reactor vessel eliminates the need for pumps. For the Brazilian FBMR, pump failure prompts an automatic reactor shutdown due to the pressure drop that secures core fluidization and prevents criticality.

Usually, the reactor is equipped with a passive heat removal system supported by active an active system. The RPV couples to at least one sink for heat removal. Reactivity is managed by control and shut down rods, together with the injection of liquid absorbers e.g. boric acid.

2.10.3 Supercritical Water Reactors

The safety systems described are based on the SuperSafe Reactor (SSR) design. The coefficient of void reactivity together with the power coefficient of reactivity are both

negative to ensure self-stability of the reactor during abnormal conditions. Therefore, peak temperature never exceeds the melting point of either the cladding or fuel. High pressure tubes are vulnerable to rupture if even small leakage occurs, and monitoring is required to ensure reactor shut down and tube depressurization. If leakage leads to tube rupture, a passive Primary Coolant Safety System (PCSS) will inject water into the reactor and equalize the loss of water.

By placing pressure tubes in the heavy water filled calandria filled at near-ambient pressure, an additional Moderator Safety System (MSS) is created. The MSS is also passive and able to remove 100% decay heat even after complete coolant loss from the primary system. This system also can stabilize and maintain decay heat for long periods.

These ideas are expanded in Chapter 5.

2.10.4 Liquid Metal Reactors

During shutdown, natural convection occurs inside the reactor vessel and excess decay heat is removed by redundant heat exchangers. The advantage of using liquid metal in an SMR is its higher heat inertia that provides more time to respond. Moreover, the coolant operates at near atmospheric pressure, and the control rods can be adjusted quickly due to the low pressure in the vessel. The possibility of LOCA is also minimized.

Safety systems in SFRs focus on the leakage prevention, and usually, the reactor is placed in a containment vessel. Generally, the reactor is a pool type to more readily integrate the primary pumps with the Intermediate Heat Exchangers (IHX). Moreover, redundant independent heat exchangers inside the vessel ensure heat removal from the core if the IHX fails. Both lead and LBE have inert chemical properties and there is little danger of explosion or fire in the event of leakage. Moreover, the coolant will solidify serve as a surface seal.

2.10.5 Gas Cooled Reactors

GCRs use fully passive systems during all events due to low power density in the RPV. Ceramic TRISO (TRIsstructural-ISOtropic) fuel elements can withstand high temperatures that may occur during accidents. Moreover, the layers of carbon and silicon carbide in the fuel retain nuclides up to 1600°C, capturing almost all radioactive fission

products during accidents. Helium is a convenient coolant as it is chemically inert and radiation insensitive.

2.11 Proliferation Considerations

Commercial nuclear reactors and enrichment infrastructures can be adapted to produce weapon grade materials and devices and steps against nuclear weapon proliferation are necessary.

Thorium based fuels protect against proliferation because thorium is a fertile, rather than a fissile, material. The fuel cycle is designed to produce enough fissile ^{233}U only for current operations with a breeding factor of around 1. Moreover, plutonium produced in this cycle has a higher content of ^{240}Pu than the uranium cycle. Since ^{233}U can be easily denaturized with natural uranium, it is harder to extract fissile material.

TRISO fuel elements consist of a graphite, silicon carbide, pyrolytic carbon and small amount of fuel material, e.g. uranium. Therefore, recovering fissile material is difficult due to a number of barriers and the number of TRISO pellets in the core can be over a hundred thousand. GCRs can burn weapon-grade material, and can contribute to non-proliferation by decreasing the amount of fissile material. Together with the difficulty of extracting fissionable material from TRISO fuel elements, GCRs secure very high proliferation resistance.

Fast reactors with breeding factors above unity can achieve long time operation without refueling. Therefore, it is possible to build a reactor that will not require refuelling for at least 5 years. Prospective designs will use ultra-long life fuel cycles, i.e. the operation period will be up to 40 years after which the reactor will be decommissioned. The use of liquid metal can create additional obstacles to proliferation, as for example, sodium may ignite should piping rupture, while lead or lead-bismuth eutectics will solidify.

Chapter 3

Methodology***

This chapter details the methodology used to perform the numerical evaluations and simulations of fluid dynamics and thermodynamics. The basic thermodynamics underlying the analytical analyses are summarised. The approach to computational fluid dynamics is described, including the differences between particular turbulent models and when it is appropriate to use these models. The rationale for selecting the numerical analysis tools is given.

*This section published substantially as reference: Rowinski et al. (2015). "Innovative model of annular fuel design for lead-cooled fast reactors." Progress in Nuclear Energy 83(0): 270-282

**This section published substantially as reference: Rowinski et al. "Numerical Investigation of Supercritical Water Flow in a Vertical Pipe under Axially Non-Uniform Heat Flux", under review in Progress in Nuclear Energy

3.1 Simulations

Two methodologies were available depending on the research problem under investigation. For 1D investigation of temperature distribution inside nuclear fuel elements an analytical-numerical approach was appropriate. The remaining research of the thermal response of supercritical flow used Computational Fluid Dynamic (CFD) analysis.

3.2 Computational Tools

The main tool deployed was the CFD software Fluent developed by ANSYS, Inc. to calculate the flow patterns by solving the Navier-Stokes equation and conservation equations of mass, momentum, and energy using the finite volume method to provide a satisfactory trade-off between accuracy and performance. It is one of the most advanced codes available and allows the simulation of 2D, 2D-axisymmetric and 3D flows in steady or unsteady and laminar or turbulent states. Parameters are customized with self-created User Defined Functions (UDFs) to correlate responses with pressure or temperature. The code is scalable on multithreaded machines and integrates the “NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)” [81] for water and carbon dioxide at sub- and supercritical conditions to be used in Generation IV nuclear reactors. Because of those capabilities. Other codes considered included:

- (i) OpenFOAM is an open source code developed by OpenCFD Ltd where a finite volume method can be customized. However, for the present project considerable coding and verification beyond the scope of the thesis was required.
- (ii) ANSYS CFX combines the control volume and finite element methods and perform flow calculations similar to ANSYS Fluent, however, the convergence and overall performance proved less successful for the current applications. The tool was originally created to perform turbomachinery calculations, but lacks a 2D solver, and only 3D or pseudo-3D cases can be calculated.
- (iii) Code_Saturn is an open source code developed by EDF. The program has a number of built-in options and is capable of performing advanced calculations. However, the user base is limited and lacks validation in supercritical flow applications.

Before performing CFD calculations, the fuel assembly geometry was created and meshed. All geometries were prepared using GAMBIT software developed by Fluent Inc. that provides good control for creating CFD geometries and together with ICEM CFD generated mesh geometries. The first software was used to mesh simple 2D models, whereas ICEM was used for meshing advanced 3D geometries of fuel bundles.

Additional software used in the research were:

- (i) Microsoft Excel to perform preliminary analysis of collected data,
- (ii) Origin to create figures and graphs, and
- (iii) JetBrains PyCharm as an interpreter of Python programming language to perform data analysis, graph creation and 1D simulations.

3.3 Technique 1 – 1D Analytical Analysis

In order to conduct an analysis of thermal parameters, it is necessary to specify known reactor parameters, calculate or estimate unknown factors, and derive relevant equations. The analysis was based on thermodynamic models with the following assumptions:

- (i) cylindrical coordinate system,
- (ii) one dimension, i.e. only $\frac{d}{dr}$,
- (iii) steady state i.e. $\frac{\partial}{\partial t} = 0$ and $q''' = \text{const}$,

3.3.1 Flow characteristics

Flow characteristics show how heat is removed from the fuel elements where the most important factors are the velocity of the medium and the cross-section area together with hydraulic diameter.

The calculation of the Reynolds number is given by:

$$\text{Re} = \frac{\rho v D_H}{\mu} \quad (1)$$

where ρ is the density [kg/m³], V the velocity [m/s], μ the dynamic viscosity [Pa s] of coolant and D_H the hydraulic diameter [m] which can be described as follows:

$$D_H = \frac{4A}{W} \quad (2)$$

with A being the cross section of flow area [m²], and W the wetted perimeter of the cross-section [m].

If s is the ratio between fuel pitch and rod diameter, then for square and hexagonal lattices, the following relations can be written, respectively:

$$\begin{cases} D_H = 2R_{c,oo} \left[\frac{4}{\pi} (s)^2 - 1 \right] \\ D_H = 2R_{c,oo} \left[\frac{2\sqrt{3}}{\pi} (s)^2 - 1 \right] \end{cases} \quad (3)$$

The Nusslet number shows how heat transfer behaves in the fluid flow with the rod bundle of a square lattice. The relation for liquid heavy metal is of the form [82]:

$$\mathbf{Nu} = 7.55(s) - 14(s)^{-5} + 0.007\mathbf{Pe}^{0.64+0.246(s)} \quad (4)$$

while for the hexagonal lattice, the relation is [83]:

$$\mathbf{Nu} = 0.047 \left(1 - e^{-3.8(s)} \right) \left(\mathbf{Pe}^{0.77} + 250 \right) \quad (5)$$

and for inner lead flow [84]:

$$\mathbf{Nu} = 5 + 0.025\mathbf{Pe}^{0.8} \quad (6)$$

In the calculations, the Peclet number ($\mathbf{Pe}$) is defined as the ratio of the advective transport rate to diffusive transport rate:

$$\mathbf{Pe} = \frac{vD_H}{\alpha} = \frac{vD_H \rho_{Pb} c_{pPb}}{k_{Pb}} \quad (7)$$

where α is the thermal diffusivity [m²/s], c_p the specific heat capacity [J/kg K], and k the thermal conductivity [W/m K]. The subscript Pb states the properties of lead.

3.3.2 Temperature distribution

The temperature distribution in a fuel element should satisfy safety limits and is dependent on the power generation inside the fuel material and the flow of coolant. The basis for thermal analyses is described by Fourier's law:

$$\vec{q}'' = -k\nabla T \quad (8)$$

where $\vec{q}''$ is the heat flux [W/m²] and ∇T the temperature gradient [K/m].

In the 1-D case, the steady state solution in a cylindrical coordinate (temperature depends on r the cylinder radius) system for eq. (8) will take the form of:

$$T(r) = -\frac{q'''r^2}{4k} + C_1 \ln r + C_2 \quad (9)$$

For a solid fuel element, the following boundary conditions are given:

$$\left. \frac{dT}{dr} \right|_{r=0} = 0 \quad \text{and} \quad T|_{r=R_{f,o}} = T_{f,o} \quad (10)$$

where $T_{f,o}$ is the fuel outer surface temperature [K], and R_o the outer radius [m].

After applying boundary conditions (10) to eq. (9) the 1-D steady-state temperature distribution in the fuel is:

$$T_f(r) = T_{f,o} + \frac{q'''R_{f,o}^2}{4k_f} \left(1 - \frac{r^2}{R_{f,o}^2} \right) \quad (11)$$

For annular fuel elements, the boundary conditions are:

$$\left. \frac{dT}{dr} \right|_{r=R_m} = 0 \quad \text{and} \quad T|_{r=R_{f,o}} = T_{f,o} \quad (12)$$

Thus, in 1-D, the steady state temperature distribution in annular fuel will be [85]:

$$T_f(r) = T_{f,o} + \frac{q'''R_{f,o}^2}{4k_f} \left(1 - \frac{r^2}{R_{f,o}^2} \right) + \frac{q'''R_m^2}{2k_f} \ln \frac{r}{R_{f,o}} \quad (13)$$

where R_m is the radius (in m) of the maximum fuel temperature (mean fuel radius, since the fuel rod is designed to have the same temperature in the internal and external channels).

For the gas gap and cladding temperature distribution, there is no heat generation and thus, in both cases, the solution will take the following form:

$$\frac{1}{r} \frac{d}{dr} \left(rk \frac{dT}{dr} \right) = 0 \quad (14)$$

Therefore, the solid fuel temperature distributions in the gas gap and cladding are respectively:

$$\begin{aligned} T_g(r) &= T_{c,oi} + \frac{q'}{2k_g} \ln \frac{r}{R_{f,o}} \\ T_c(r) &= T_{c,oo} + \frac{q'}{2k_c} \ln \frac{r}{R_{c,oi}} \end{aligned} \quad (15)$$

In the case of the temperature at the cladding and coolant interface, Newton's law of cooling requires that:

$$q'' = k\Delta T \quad (16)$$

Therefore, for the “hot” rod, the interface temperature will be:

$$T_{c,oo} = T_{pb} + \frac{q'}{2\pi r_{c,oo} h} \quad (17)$$

In the case of the annular fuel rod, the additional parameters γ_o and γ_i , are introduced as the outer and inner ratios of heat transfer surface area to the total heat transfer surface area, respectively. These are described as follows:

$$\begin{aligned} \gamma_o &= \frac{2\pi R_{f,o} L}{2\pi (R_{f,i} + R_{f,o}) L} = \frac{R_{cf,o}}{R_{f,i} + R_{f,o}} \\ \gamma_i &= \frac{2\pi R_{f,i} L}{2\pi (R_{f,i} + R_{f,o}) L} = \frac{R_{f,i}}{R_{f,i} + R_{f,o}} \end{aligned} \quad (18)$$

Therefore, eq. (15) for the annular fuel:

$$\begin{aligned}
T_{g,oo}(r) &= T_{C,oi} + \gamma_o \frac{q'}{2k_g} \ln \frac{r}{R_{f,o}} \text{ and } T_{g,io}(r) = T_{C,io} + \gamma_i \frac{q'}{2k_g} \ln \frac{r}{R_{g,i}} \\
T_{c,oo}(r) &= T_{C,oo} + \gamma_o \frac{q'}{2k_c} \ln \frac{r}{R_{c,o}} \text{ and } T_{c,io}(r) = T_{C,ii} + \gamma_i \frac{q'}{2k_c} \ln \frac{r}{R_{c,i}}
\end{aligned} \tag{19}$$

The temperature of the interfaces for the annular fuel will be similar to eq. 18:

$$T_{c,oo} = T_{pb} + \gamma_o \frac{q'}{2\pi r_{c,oo} h} \text{ and } T_{c,ii} = T_{pb} + \gamma_i \frac{q'}{2\pi r_{c,ii} h} \tag{20}$$

The predicted temperature distributions in the solid and annular fuels are shown in Fig. 3-5 with the maximum temperature estimated to be at the mean radius (R_m) of the fuel.

Fig. 3-1 Predicted temperature distribution in solid (a) and annular (b) fuel element

3.3.3 Pressure drop

The pressure drop calculations are based on experimental investigations [86] examining pressure drops with different spacer grids in solid and annular fuel rod assemblies where water was the medium. Plain and twist-vane spacers were used for annular fuels, and plain, split-vane and hybrid vane spacer grids for solid fuel rods in a square lattice. The present evaluation concerned the plain spacer grid in both annular and solid fuels.

The pressure drop in the inner channel was determined according to the relation:

$$\Delta P_{Ch,in} = f \frac{L_{Tot} \rho v^2}{2D_H} \tag{21}$$

where L_{Tot} is the total length of the fuel rod, and f the friction coefficient for inner flow is from the McAdams correlation and depends on the Reynolds number, i.e. the inertial to viscous forces in the fluid flow [86]:

$$f = 0.184 \mathbf{Re}^{-0.2} \quad (22)$$

For the fuel lattice, the friction coefficient is:

$$\begin{cases} f = 0.177 \mathbf{Re}^{-0.224}; & \text{for } s = 1.08 \\ f = 0.214 \mathbf{Re}^{-0.215}; & \text{for } s = 1.35 \end{cases} \quad (23)$$

The above expressions are for annular fuel and for solid fuel, respectively, derived from the experimental results using data regression process.

One must take into consideration the influence of spacer grids in the case of pressure drop calculations. Therefore, it is necessary to introduce the pressure loss coefficient at the spacer grid K_{SG} . In the aforementioned article [86] the following relations were found:

$$\begin{cases} K_{SG} = 3.682 \mathbf{Re}^{-0.172}; & \text{for } s = 1.08 \\ K_{SG} = 3.02 \mathbf{Re}^{-0.0746}; & \text{for } s = 1.35 \end{cases} \quad (24)$$

Therefore, the pressure drop in the outer channels will take the form of:

$$\Delta P_{Ch,out} = f \frac{L_{Tot} \rho v_{out}^2}{2D_H} + n K_{SG} \rho v_{out}^2 \quad (25)$$

where n is a number of spacer grids.

In the case of annular fuel rod bundles, the pressures in the inner and outer channels are the same and the mass flow rates are balanced. Thus, the following relations are needed:

$$\begin{cases} \Delta P_{Ch,in} - \Delta P_{Ch,out} = f \frac{L_{Tot} \rho v_{in}^2}{2D_H} - \left(f \frac{L_{Tot}}{2D_H} + n K_{SG} \right) \rho v_{out}^2 = 0 \\ N_{el} \dot{m}_{in} + \dot{m}_{out} = \dot{m} \end{cases} \quad (26)$$

where N_{el} and $\dot{m}$ are the number of elements in the fuel assembly and the total mass flow rate, respectively.

3.4 Technique 2 - CFD

The computational fluid dynamics (CFD) based on the Navier-Stokes equation cannot be solved analytically for all flow patterns. Therefore, numerical methods are used in the form of equation sets derived from the governing equations and solved iteratively.

3.4.1 Governing Equations

The fluid mechanics is based on three fundamental principles, namely the laws of conservation of mass, momentum, and energy.

Mass conservation

For mass conservation, the sum of mass flow at the inlets must be equal mass flow of all the outlets such that:

$$\frac{d\rho}{dt} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (27)$$

where ρ is the density, t the time, and $\mathbf{v}$ the velocity vector.

Momentum conservation

The momentum conservation based on Newton's second law, states that the acceleration of an object is dependent upon the net force acting upon the object and the mass of the object in the form of the differential equation:

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v} \mathbf{v} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} \quad (28)$$

where p is the pressure, $\boldsymbol{\tau}$ the shear stress vector, and $\mathbf{g}$ the gravity acceleration vector.

Energy conservation

Energy conservation from the first law of thermodynamics states that the total energy of the isolated system is constant. In the case of fluid volume, it is represented by:

$$\frac{dE_T}{dt} = q - P \quad (29)$$

where E_T is the total energy of the fluid including potential and kinetic energy, q the heat added to the control volume per unit time, and P the work done by the system per unit time.

The corresponding energy conservation equation in differential form can be expressed as:

$$\frac{\partial \left[\left(e_l + \frac{1}{2} v^2 \right) \rho \right]}{\partial t} + \nabla \cdot \mathbf{v} \rho \left(e_l + \frac{1}{2} v^2 \right) = -\nabla \cdot \mathbf{q}'' + \mathbf{g} \cdot \mathbf{v} \rho - \nabla \cdot \mathbf{v} p + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}) + q''' \quad (30)$$

where e_l is the internal specific energy, $\mathbf{v}$ the velocity vector, and q'' the heat flux.

Reynolds Averaging

The aforementioned equations give the instantaneous values in the Navier-Stokes equations, however, it is more convenient to solve the averaged equations. To do so, the velocity is expressed as:

$$u_i = \bar{u}_i + u_i' \quad (31)$$

where u_i is the instantaneous value of velocity, $\bar{u}_i$ the average value of velocity, and u_i' the fluctuation velocity component. The other scalar quantities are

$$\phi_i = \bar{\phi}_i + \phi_i' \quad (32)$$

where ϕ denotes other scalars such as pressure, energy, etc.

Substituting eq. 31 into the instantaneous mass conservation equation (Eq. 27) yields:

$$\frac{d\rho}{dt} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \quad (33)$$

and substituting eq. 31 into instantaneous momentum equation (Eq. 28) gives:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] + \frac{\partial}{\partial x_j} (-\overline{\rho u_i u_j}) \quad (34)$$

The term $-\overline{\rho u_i u_j}$ is so-called Reynolds stress and must be modelled in order to close equation 28.

3.4.2 Turbulence models

Turbulent models fall into many categories, but the most important consideration is the trade-off between computation time and accuracy, and ideally, the algorithm should be accurate and efficient/fast. As these requirements are rarely met simultaneously, complex turbulent flow calculations have an accuracy dependent on how many parameters are taken into account. Common turbulent models used in CFD codes are described below based on the ANSYS Theory Guide [87, 88].

k – ε Turbulent Model:

The $k – \varepsilon$ turbulent semi-empirical two-equation model is commonly used and is based on the transport equation model of turbulence kinetic energy as a trace of the Reynolds stress $k = \frac{1}{2} \overline{u'_i u'_i}$ [m² / s²] and its dissipation rate $\varepsilon_{ij} = \frac{2}{3} \delta_{ij} (\rho \varepsilon + Y_M)$ [m² / s³]. The turbulence kinetic energy k and dissipation rate ε are obtained from the transport equations:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b + \rho \varepsilon - Y_M + S_k \quad (35)$$

and

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \quad (36)$$

where G_k is the generation of turbulence kinetic energy [kg/m s²] due to mean velocity gradients, G_b the generation of turbulence kinetic energy due to buoyancy [kg/m s²], Y_M the contribution to fluctuation dilatation incompressible turbulence to the overall dissipation rate [kg/m s²], $C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$ are constants determined from experiments with

air and water, σ_k and σ_ε the turbulent Prandtl numbers for k and ε , respectively, and S_k and S_ε are user-defined source terms.

This model is only valid for fully turbulent flows. It is possible to distinguish three versions of the $k - \varepsilon$ model and the differences are in accuracy for different types of flow, e.g. low and high Reynolds numbers.

k - ω Turbulent Model:

The standard $k - \omega$ turbulent two-equation empirical model developed by Wilcox [89] predicts the free shear flow spreading rates based on transport equations for turbulence kinetic energy (k) and the specific dissipation rate (ω) [1/s], which is a ratio of ε and k :

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}(\Gamma_k \frac{\partial k}{\partial x_j}) + G_k - Y_k + S_k \quad (37)$$

and

$$\frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho \omega u_i) = \frac{\partial}{\partial x_j}(\Gamma_\omega \frac{\partial \omega}{\partial x_j}) + G_\omega - Y_\omega + S_\omega \quad (38)$$

where G_k is the generation of turbulence kinetic energy due to mean velocity gradients, G_ω the generation of ω [kg/m s²], Y_M and Y_ω are dissipation of k and ω [kg/m s²], Γ_M and Γ_ω are effective diffusivity of k , and ω , S_k and S_ε are user-defined source terms.

The $k - \omega$ predicts with sufficient accuracy all near wall effects, since it does not use any wall functions, while the flow in the free stream is less accurate.

Shear-Stress Transport (SST) k - ω model:

The SST model was developed to combine the accurate prediction of $k - \omega$ in the near wall region with the performance of the $k - \varepsilon$ turbulent model in the free stream in the far field of the flow. This is accomplished by converting the $k - \varepsilon$ model into the $k - \omega$ model by a multiplicative blending function and summation. Hence, the blending function is unity in the near-wall region in order to use the $k - \omega$ model, and zero away from the surface where the $k - \varepsilon$ model is used. It can be concluded that the SST $k - \omega$

model combines $k - \omega$ and $k - \varepsilon$ in order to provide accurate results both at the near wall and in the free stream, and appropriate for a wider spectrum of applications. Moreover, Wen and Gu [90] and Kao et al. [91] validated several turbulent models against supercritical flows and concluded that the SST $k - \omega$ models are the most accurate.

Other Turbulent Models:

The turbulent models below were not used because the SST $k - \omega$ turbulent model proved satisfactory. However, brief descriptions of these models are provided here:

- (i) The Spalart-Allmaras model is a one-equation model for the kinematic eddy (turbulent) viscosity. It is the fastest turbulent model developed for aerospace applications and has limited application in turbomachinery.
- (ii) The Reynolds Stress Model (RSM) is a five-equation model for 2D and a seven-equation model for 3D. It solves the Reynolds stresses, together with an equation for the dissipation rate. In this approach computation time increases significantly while the results differ little from the much faster two-equation models.
- (iii) The Large Eddy Simulation (LES) model solves large eddies directly, while small eddies are modeled using the turbulent model. It is applicable only to 3D cases, and the computation time and system requirements are of an order of magnitude larger than typical RANS models.
- (iv) The Direct Numerical Simulation (DNS) solves all turbulences directly and currently it is unsuitable for complex flow due the large computational requirements. Only simple geometries with low Reynolds numbers are feasible presently, and these are not appropriate for the current investigation.

Chapter 4

Innovative Model of Annular Fuel Design for Lead-Cooled Fast Reactions*

Analytical solutions of the default (solid fuel) and innovative (annular fuel) approaches are described with the latter showing promise in terms of safety. As liquid metal cooled reactors burn reprocessed fuel or processed weapon-grade plutonium high safety standards must be assured. Here, seven square and hexagonal annular fuel assemblies were examined, with the effect of spacer grids taken into consideration. It was shown that the annular fuel reduces maximum fuel temperature by up to 757°C in comparison to the default base design including spacer grids. The most promising design is a hexagonal lattice with 91 fuel elements and an 18×18 square lattice, where the maximum temperatures are 822°C and 732°C, while pressure drops are 185 kPa and 128 kPa, respectively. The square lattice proved superior in this evaluation, with similar or smaller pressure drops than the reference solid fuel design. This opens the possibility of using smaller coolant pumps in the case of annular fuel elements. Moreover, the annular fuel allows reactor overpowering to 110% of the nominal power, while securing all safety limits. It is concluded annular fuels are a promising concept requiring further investigation.

*This section published substantially as reference: Rowinski et al. (2015). "Innovative model of annular fuel design for lead-cooled fast reactors." Progress in Nuclear Energy 83(0): 270-282

4.1 Introduction

The constant growth in energy demand will require, in addition to building new power plants, improvements in efficiency. Therefore, the production of the same amount of energy will require fewer resources, and be friendlier to the environment. The simplest way to increase the overall efficiency is to improve the performance of a nuclear power plant (NPP) is to design new fuel element assemblages.

Currently, NPP use solid fuel elements due to their proven reliability. Although state-of-the-art, there are inefficiencies in heat exchange between the heat source and coolant. Hence, Kazimi et al. [92] proposed the annular fuel rods will show better performance than the default solid fuel pin design. The United States of America conducted independent feasibility studies for water and Sodium-cooled Fast Reactors (SFRs) [93-95], while South Korea evaluationed for water and gas-cooled reactors [86, 96-100]. The temperature distribution is much less in annular fuel elements, while the pressure drop along the channel can be minimized by optimizing the fuel assembly geometry. Similar studies of annular fuel in Lead-cooled Fast Reactors (LFRs) are not available.

The main difference between annular fuel and solid fuel is that the former allows coolant to flow not only in a gap between fuel rods, but also through the element itself. Internal and external cooling provides a larger heat exchange area and superior fuel performance. Thus, the power density is higher and the amount of heavy metal in the reactor core can be decreased while the overall power will be the same or higher. Concomitantly, the maximum temperature in the fuel will decrease significantly, providing higher safety margins in the case of emergency conditions. On the other hand, an increase of cladding may lead to a slightly higher enrichment of the fuel due to additional parasitic absorption.

As discussed in Chapter 2 several Generation IV reactors are in design or development:

- (i) SuperCritical Water-cooled Reactors (SCWRs) [101-104].
- (ii) Liquid metal fast reactors that can be further divided into:
 - a. Sodium-cooled Fast Reactors (SFRs) [40, 105, 106].
 - b. Lead-Cooled Fast Reactors (LCFRs) [78, 107-109].
- (iii) Gas-cooled Fast Reactors (GFRs) [48, 49, 97].

The LCFR was chosen for further analysis due to its coolant properties, characterized by a very high boiling point¹ at normal pressure, and low reactivity with water and/or air. Moreover, in the case of leakage, lead will solidify. This together with the relatively low melting temperature², low moderation ability, allows capture of iodine and cesium in the event of radioactive leakage from fuel elements to the coolant.

Generally, the fuels proposed for Generation IV reactors are plutonium-uranium nitride or plutonium-uranium oxide fuel, and in order to flatten the neutron flux distribution in the core, different plutonium enrichment zones are introduced. Two fuel lattice designs are investigated, i.e. open square and closed hexagonal [78-80].

4.2 Methods

As described in Chapter 3 the calculations are divided into five parts from specification of the fuel concept and reactor parameters, through to the design process, to the analysis of thermal parameters and pressure drop.

4.2.1 The fuel concept

The ordinary nuclear fuel has the form of solid fuel pins, surrounded usually, by a zircalloy cladding with good neutronic properties and a gap of inert gas between fuel pins and cladding. The solid and annular fuel designs are compared in Fig. 4-1.

Solid fuel was modelled for both hexagonal and square lattices as a reference for further analysis (Fig. 4-2). The main limitations regarding of lead as a coolant are the maximum fluid velocity, due to the erosion of cladding material, and the maximum cladding surface temperature (MCST), due to the corrosiveness of lead in high temperature.

Based on the dimensions of the solid fuel assembly, reactor properties, and coolant to fuel volume ratio, the annular fuel assemblies were created (Fig. 4-3). The gas gap and cladding thicknesses are the same in every design, thus annular fuel must contain less fuel and more cladding material in the fuel assembly.

¹ Boiling point: a) lead – 1737°C, b) LBE – 1670°C

² Melting point: a) lead – 327°C, b) LBE – 125°C

Fig. 4-1 Comparison of default solid fuel (left) and proposed annular fuel (right)

Fig. 4-2 Scheme of default assembly lattices a) square b) hexagonal [78]

Fig. 4-3 Schemes of proposed assembly lattices a) square b) hexagonal

In order to achieve near identical reactor performance, the coolant to fuel ratio is the same for every design, thus a new parameter δ , the coolant-to-fuel volume ratio, was introduced equal to 1.676 and 1.842 in the case of square and hexagonal lattices, respectively. Moreover, another parameter β , which is the ratio between the reference and particular fuel volumes, is always less than unity.

The lattice design scheme includes the following dimensions presented in Fig. 4-4:

- (i) outer element radius – $R_{c,oo}$,
- (ii) inner element radius – $R_{c,ii}$,
- (iii) pitch between fuel rods – p ,
- (iv) the length of the lattice side (square) – a , or radius of circumscribed circle of the hexagon – R , which are constant parameters.

Fig. 4-4 Dimensions of the fuel elements

4.2.2 Reactor parameters

The European Lead System (ELSY) reactor is in development under the Sixth EURATOM Framework Programme by Ente Nazionale per l'Energia Atomica (ENEA), the Nuclear Research and Consultancy Group (NRG), and Centre national de la recherche scientifique (CNRS), the Royal Institute of Technology (KTH), Sweden and AGH University of Science and Technology, Poland [43]. Table 4-1 presents the most important parameters of the reactor. Since the prediction suggests superior cooling ability, the calculations were also conducted in the case of a 110% reference power value, shown in parentheses.

Table 4-1 Main ELSY reactor's parameter [78]

Parameter	Value	
Power [MW _{th}]	1500 (1650)	
Inlet temperature [°C]	400	
Outlet temperature [°C]	480	
Maximum allowed clad surface temperature [°C]	550	
Maximum fluid velocity [m s ⁻¹]	2	
Core's active length [m]	1.2	
Total length of fuel element [m]	2.5	
Type of lattice	Square	Hexagonal
Number of fuel assemblies	162	427
Number of elements per assembly	441	169
Element pitch [mm]	13.9	15.5

For annular fuels an increase of cladding material may lead to higher parasitic absorption and degrade performance, requiring evaluation with respect to fuel enrichment. Memmott et al. [95] conducted an evaluation of SFR and found annular elements require slightly more enriched fuel that decreases the conversion ratio leading greater burn-up than solid fuel. This property would prove advantageous for burning reactors.

4.2.3 Material properties

The coolant properties, i.e. isobaric specific heat, dynamic viscosity, thermal conductivity and density of coolant are estimated at a mean fluid temperature of 440°C according to the relations from [84] (Table 4-2). The thermal conductivity of UO₂ is estimated to be 2.9 W/m K at 1000°C [110], while the cladding thermal conductivity at 525°C is taken from the ASME standard [111] for austenitic steel AISI 316 L, which is the candidate for cladding material for LMCR.

Table 4-2 Properties of lead at 0.1MPa [84]

Property	Equation	Temperature Range [K]	SI Unit	Estimated Error
Density	$\rho_{pb} = 11367 - 1.1944T$	601-1900	Kg/m ³	0.7%
Dynamic viscosity	$\mu_{pb} = 4.55 \times 10^{-4} \exp\left(\frac{1069}{T}\right)$	601-1470	Pa s	4%
Thermal conductivity	$k_{pb} = 9.2 + 0.011T$	601-1300	W/m K	10%
Isobaric specific heat	$c_{p_{pb}} = 175.1 - 4.961 \times 10^{-2}T + 1.985 \times 10^{-5}T^2 - 2.099 \times 10^{-9}T^3 - 1.524 \times 10^6 T^{-2}$	601-1300	J/kg K	7%

Thermal conductivity of the gas gap is 0.9 W/m K_q calculated according to Kazimi [93]:

$$k_g = h_g R_g \ln \left(\frac{R_{c,oi}}{R_{f,o}} \right) \quad (39)$$

where gas conductance h is taken as 6,000 W/m² K and typical for a fuel element.

4.2.4 Material limitations

The Lead-bismuth eutectic (LBE) was used as a coolant in Russian submarines without major accidents and is of proven reliability [33, 112-114]. However, the main disadvantages of lead and LBE are corrosiveness at high temperatures which limits the maximum cladding surface temperature (MCST) to 550°C, especially in the case of LBE,

since bismuth boosts the corrosive properties of the coolant. It was found that the austenitic and martensitic steels are able to withstand temperatures up to 550°C in the lead environment if sufficient oxygen control is provided [115]. Müller et al. [116] conducted tests with the use of austenitic stainless steels such as AISI 316L, 1.4970 and MANET and concluded all can withstand temperatures of up to 550°C for 4000 hours. Surface coating with Al alloy prevents corrosion to 600°C in the lead medium. Hence, a conservative estimate will limit MCST to 550°C.

The literature suggests that cladding strain due to mechanical interactions between the fuel and cladding will be minimal during steady-state operation, as the oxide fuel is plastic under irradiation, especially by irradiation-induced creep, although carbide based fuels are more rigid [117]. Other difficulties are the opaqueness of the lead medium and its erosive properties that limits coolant velocity to 2 m s⁻¹. For LBE there is a higher production of polonium-210 (²¹⁰Po) from bismuth making pure lead a more reasonable option. According to Zinkle et al. [118], the high energetic neutron flux will accelerate the degradation of the material, due to void swelling and phase instability during irradiation. Therefore, research for suitable cladding alloys is ongoing.

4.3 The Design Process

The main design challenge is to ensure the pressure drop in the inner and outer channels is always balanced. As the fuel assembly should allow easy replacement of the solid pins by annular elements, the only variables are the inner radius and outer cladding diameters together with the pitch between fuel elements. The number of fuel elements will be smaller due to the larger external radius in annular fuel to accommodate the inner channel. All relations described earlier are adjustable and an optimizing function written. Changing the number of elements per assembly sets the dimensions for the fuel element.

4.4 Results and Discussion

Calculations were undertaken with and without spacer grids inside the fuel assembly, in order to better understand the phenomena occurring in annular fuel. The temperature distribution calculations were performed for the “hot” rod in the lattice where the temperature distribution is the highest and the chance of failure largest. Moreover, the calculations were conducted for normal and maximum-possible overpower conditions,

which was estimated to be 10%. The core radial and axial peaking factor were taken from [79], i.e. radial peaking factor of 1.14 and axial peaking factor of 1.24 where neutronic calculations were performed for the default solid fuel and square fuel lattice. Since the fuel assembly dimensions and coolant to fuel volume ratio are the same, the peaking factors are assumed valid for all designs, including solid and annular fuel. The pressure drop calculations were performed for the whole fuel assemblies.

4.4.1 Assembly without spacers

For rod bundles without spacer grids the dimensions of models are found in Tables 4-3 and 4-4 for the square and hexagonal lattices, respectively. The pitch to element diameter (s) is similar to annular fuel, and for the square lattice, is around 1.075 which is similar to the experimental value of 1.08 found by Lee et al. [98]. Hence, the pressure drop correlations are valid. For the hexagonal lattices it is around 1.227.

Table 4-3 Input parameters for square lattice calculations

	$R_{c,oo}$ [cm]	$R_{c,oi}$ [cm]	$R_{f,o}$ [cm]	$R_{f,i}$ [cm]	$R_{c,io}$ [cm]	$R_{c,ii}$ [cm]	s [cm]
Solid_21	5.25	4.65	4.5	N/A	N/A	N/A	1.323
Annular_19	7.18	6.58	6.43	4.39	4.24	3.64	1.070
Annular_18	7.56	6.96	6.81	4.64	4.49	3.89	1.073
Annular_17	7.99	7.39	7.24	4.91	4.76	4.16	1.075
Annular_16	8.47	7.87	7.72	5.22	5.07	4.47	1.077
Annular_15	9.02	8.42	8.27	5.57	5.42	4.82	1.079

Table 4-4 Input parameters for triangular lattice calculations

	$R_{c,oo}$ [cm]	$R_{c,oi}$ [cm]	$R_{f,o}$ [cm]	$R_{f,i}$ [cm]	$R_{c,io}$ [cm]	$R_{c,ii}$ [cm]	s [cm]
Solid 169	5.3	4.7	4.55	N/A	N/A	N/A	1.462
Annular 127	7.31	6.71	6.56	4.22	4.07	3.47	1.222
Annular 91	8.56	7.92	7.81	4.97	4.82	4.22	1.231

Figure 4-5 plots the parameters that affect neutronics and thermal-hydraulics performance for both square (left) and hexagonal (right) lattices. The annular assembly

contains less fuel than the solid one as the amount of varies cladding material is inversely. consequently, the normalized amount of fuel to the default design is always lower than unity and decreases with the number of rods, while the cladding material is above unity and increasing. From a neutronics point of view, a greater number of fuel elements leads to a higher parasitic absorption in the claddings. Nevertheless, the cooling surface area is much greater, i.e. in the worst case, the cooling surface area is 2.4 times larger, which is a great advantage over solid fuel. It is shown that the cooling surface area is up to 3.08 and 3.57 times greater for square and hexagonal lattices, respectively.

Fig. 4-5 Key parameters normalized to the default designs

Table 4-5 compiles the maximum power density and linear power density for different square lattice models. Because the reactor power is constant, but the number of fuel elements differ in each design, all of the values are for the reference power output of 1500 MW_{th}. The ratio of maximum linear power density per fuel element is up to 196% of the reference for the annular approach, and decreases with the number of fuel elements. Nevertheless, the power density ratio behaves proportionally to the number of power rods. The highest value in comparison to the solid fuel is only 12% higher.

Table 4-5 Maximum power density and linear power density per fuel element in square lattice

	Total number of fuel elements	δ	β	Ratio between particular and reference power density	Ratio between particular and reference linear power density
Solid_21	71442	1.676	100%	100%	100%
Annular_19	58482	1.676	88.98%	112.4%	122.2%
Annular_18	52488	1.676	90.21%	110.9%	136.1%
Annular_17	46818	1.676	91.45%	109.4%	152.6%
Annular_16	41472	1.676	92.70%	107.9%	172.3%
Annular_15	36450	1.676	93.95%	106.4%	196%

In the case of the hexagonal lattice, the ratio of maximum power density per annular fuel element is up to 9% higher than for the solid fuel approach, but for the linear power density ratio, the value is up to 185% that of the reference solid fuel (Table 4-6). The behaviour of those parameters is similar to the square lattice.

Table 4-6 Maximum power density and linear power density per fuel element in hexagonal lattice

	Total number of fuel elements	δ	β	Ratio between particular and default power density	Ratio between particular and default linear power density
Solid 169	72163	1.842	100%	100%	100%
Annular 127	54229	1.842	91.68%	109%	133%
Annular 91	38857	1.842	94.49%	105.8%	185.7%

4.4.1.1 Temperature distribution

The base design is characterized by the highest temperature distribution inside the fuel element. Figure 4-6 compares the standard solid fuel element and the annular design for the square lattice with the latter superior in terms of temperature distribution, where the maximum temperature is over 700°C lower than in base fuel design. The overall temperature decreases with an increase of the fuel elements, even though the temperature of the interface between cladding and coolant is constant at 513°C. The maximum temperature of the annular fuel in the 15×15 lattice is 786°C. The smallest is in the 19×

19 lattice, at 707°C, while the centreline temperature of the solid element is more than double at 1473°C. The dashed lines show values of a 10% overpowered reactor.

Fig. 4-6 Temperature distribution in various square lattices

Figure 4-7 shows the temperature distribution in the hexagonal fuel lattice. Again, the base solid element design is characterized by the highest temperature while the annular fuel designs rise to about 700°C. The coolant temperature is the same in every case but the spread is less for the annular fuel. The temperature decreases with the number of fuel rods in the assembly. The maximum temperature of the annular fuel is in lattice 91 (788°C) and the smallest is in the lattice 127 (725°C), while the solid element reaches 1461°C. As expected, the temperatures are slightly higher in the square lattices with annular elements, due to the compact geometry. The dashed lines show the overpowered reactor.

The overpower (110%) calculations found temperature distributions (dashed lines) only slightly higher than in the 100% power level case; nevertheless, a higher rise in the power output exceeds the limit for coolant velocity in the square lattice. Hence, to keep the same temperature at the coolant to cladding interface at the velocity limit, power uprating beyond 10% is not recommended for the hexagonal lattice.

4.4.1.2 Pressure drop

Pressure drop is another important property, as it is the key parameter when selecting pump power. Figure 4-8 presents the pressure drop in different lattices.

Fig. 4-7 Temperature distribution in various hexagonal lattices

Fig. 4-8 Pressure drop (kPa) in square (a) and hexagonal (b) lattices

The pressure drop in square and hexagonal lattices increases with the number of fuel rods, due to smaller outer flow area, thus smaller hydraulic diameter. For both inner and outer flows, the value is higher than for the base design in this case. The pressure drop is lower for the base hexagonal lattice, while for annular elements the pressure drop is lower in the square lattice.

4.4.2 Assembly with spacers

Calculations for the fuel assemblies with spacer grids were performed in the same manner with the same number of elements per fuel assembly. The element dimensions were adjusted to obtain a balance between inner and outer pressure loss in the elements since the pressure drop will be higher in the presence of spacer grids. Tables 4-7 and 4-8 show that the dimensions of the fuel rods are slightly smaller than in the case without spacers. Therefore, the results differ from the previous case.

Table 4-7 Input parameters for square lattice calculations with spacers

	$R_{c,oo}$ [cm]	$R_{c,oi}$ [cm]	$R_{f,o}$ [cm]	$R_{f,i}$ [cm]	$R_{c,io}$ [cm]	$R_{c,ii}$ [cm]	s [cm]
Solid_21	5.25	4.65	4.5	N/A	N/A	N/A	1.323
Annular_19	7.02	6.42	6.27	4.13	3.98	3.38	1.095
Annular_18	7.38	6.78	6.63	4.34	4.19	3.59	1.099
Annular_17	7.79	7.19	7.04	4.58	4.43	3.84	1.103
Annular_16	8.24	7.64	7.49	4.84	4.69	4.09	1.107
Annular_15	8.75	8.15	8	5.13	4.98	4.38	1.112

Table 4-8 Input parameters for triangular lattice calculations with spacer

	$R_{c,oo}$ [cm]	$R_{c,oi}$ [cm]	$R_{f,o}$ [cm]	$R_{f,i}$ [cm]	$R_{c,io}$ [cm]	$R_{c,ii}$ [cm]	s [cm]
Solid 169	5.3	4.7	4.55	N/A	N/A	N/A	1.462
Annular 127	7.08	6.48	6.33	3.80	3.65	3.05	1.262
Annular 91	8.23	7.63	7.48	4.38	4.23	3.63	1.280

Fig. 4-9 shows that for fuel assembly with spacer grids, the cooling surface is slightly lower than without spacers (Fig. 4-5). The assembly with the highest number of fuel rods has a cooling area 2.31 times that of the reference design, while the highest value is 2.92 or 3.35 times greater than for square or hexagonal lattice, respectively. The remaining parameters are negligibly different from the case without spacers.

Table 4-9 compiles the maximum power density and linear power density for different models in square lattices at 100% power output. The ratio of linear power density per fuel element is the same as in the previous case, i.e. 196% of the value of the solid fuel

element. Nevertheless, the highest value in comparison to the solid fuel is only 11% higher, thus slightly lower than in the case without spacers.

Fig. 4-9 Key parameters normalized to the default design (with spacers)

Table 4-9 Maximum power density and linear power density per fuel element in square lattice (with spacers)

	Total number of fuel elements	δ	β	Ratio between particular and default power density	Ratio between particular and default linear power density
Solid_21	71442	1.676	100%	100%	100%
Annular_19	58482	1.676	89.94%	111.2%	122.2%
Annular_18	52488	1.676	91.18%	109.7%	136.1%
Annular_17	46818	1.676	92.43%	108.2%	152.6%
Annular_16	41472	1.676	93.69%	106.7%	172.3%
Annular_15	36450	1.676	94.95%	105.3%	196%

Table 4-10 Maximum power density and linear power density per fuel element in hexagonal lattice (with spacers)

	Total number of fuel elements	δ	β	Ratio between particular and default power density	Ratio between particular and default linear power density
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Solid 169	72163	1.842	100%	100%	100%
Annular 127	54229	1.842	92.94%	107.6%	133.1%
Annular 91	38857	1.842	95.76%	104.4%	185.7%

In the case of the hexagonal lattice (Table 4-10), the linear power density ratio is up to 185% that for solid fuel, while the maximum power density ratio per fuel element is slightly smaller at 7.6% higher, due to the smaller dimensions of the fuel and higher β , which defines the amount of fuel in the assembly.

4.4.2.1 Temperature distribution

The slightly different size of the fuel elements slightly increases the temperature distribution inside the fuel rods with spacers. Figure 4-10 presents results for square lattices. The maximum temperature is more than 700°C lower than the base fuel design. The highest temperature for the annular fuel is found in lattice 15×15 to be 806°C, and the lowest is in the lattice 19×19 at 715°C, while the temperature of the solid element reaches 1472°C.

Fig. 4-10 Temperature distribution in various square lattices (with spacers)

Figure 4-11 shows the temperature distribution in the hexagonal fuel lattice. Again, the maximum temperature of the solid element design is highest while the annular fuel is more than 700°C lower. The highest temperature of the annular fuel is in the lattice of 91

fuel elements (823°C), and the lowest is in the lattice of 127 (747°C), while the temperature of the solid element is 1461°C. Again, hexagonal lattices operate at higher temperatures than the square lattice.

Fig. 4-11 Temperature distribution in various hexagonal lattices (with spacers)

The temperature distribution at 110% power output (dashed lines), as for the case without spacers, shows temperatures are slightly higher than the default case. The maximum temperature difference in annular fuel is about 20°C, while for solid fuel it is nearly 100°C more than in the nominal power output. Again, the hexagonal lattice does not allow any overpowering of the reactor (Fig. 4-11 – dashed lines).

Fig. 4-12 Pressure drop (kPa) in square (a) and hexagonal (b) lattices in the outer channels in annular fuel (with spacers)

4.4.2.2 Pressure drop

The correlations between pressure drops in the solid pin and annular approaches are distinct (Figure 4-12). The pressure drop sum across the outer channel and the influence of the spacer grids must be equal to the pressure drop in inner channel, i.e. ΔP_{total} is equal to ΔP_{inner} . The pressure drop in square and hexagonal lattice increases with a number of fuel rods in assembly. In the case with spacer grids, only one square lattice approach design has higher pressure drop than the default, which is desirable. The share of pressure drop related to grid spacers decreases significantly to almost half the reference case.

The pressure drop in the hexagonal lattice always exceeds the annular design (Fig. 3-13b). A further reduction in the number of fuel elements would decrease the pressure drop, but also increase the interior temperature of the fuel element. This is important as the temperatures are already higher than the square lattice. Hence, the hexagonal lattice shows less desirable properties and is an unsuitable candidate for further evaluation.

Such behaviour arises because the pressure drop in the inner channels must balance the pressure drop in the outer channels, and consequently the sum of pressure drops related to the friction factor and spacer grids. Therefore, to obtain a higher pressure drop in the inner channel, the hydraulic diameter must be smaller than in the case without spacers, as the pressure drop and inner radius are inversely proportional. A smaller number of fuel elements in the assembly would increase the inner rod hydraulic diameter, but the temperature distribution would increase with this configuration.

The main contributor to the pressure drop in case of annular flow is the length of the fuel rod, as friction acts on a large area due to the greater size of fuel elements and decreases rapidly with number of fuel rods. The grid spacer effect is smaller and the pressure decreases more slowly.

Table 4-11 Pressure loss characteristics in square lattice (with spacers)

	Delta P_{Ch}	Delta $P_{K\ SG}$	Delta P_{total}	f_{in}	f_{out}	K_{SG}	$\dot{m}_{in}$	$\dot{m}_{out}$	$\dot{m}_{total}$
Solid_21	47.215	84.840	132.055	N/A	0.0181	0.8974	N/A	1	128371
Annular_19	78.929	60.375	139.304	0.0147	0.0200	0.5460	0.325	0.675	128371

Annular_18	70.146	57.794	127.940	0.0146	0.0198	0.5409	0.327	0.673	128371
Annular_17	62.049	55.270	117.318	0.0144	0.0196	0.5356	0.329	0.671	128371
Annular_16	54.594	52.797	107.391	0.0142	0.0193	0.5299	0.332	0.668	128371
Annular_15	47.745	50.369	98.114	0.0140	0.0191	0.5240	0.334	0.666	128371

Table 4-12 Pressure loss characteristics in hexagonal lattice (with spacers)

	Delta P_{Ch}	Delta P_{K_SG}	Delta P_{total}	f_{in}	f_{out}	K_{SG}	$\dot{m}_{in}$	$\dot{m}_{out}$	$\dot{m}_{total}$
Solid 169	31.97	65.94	97.92	N/A	0.0176	0.8987	N/A	1	128371
Annular 127	105.83	122.52	228.35	0.0123	0.0196	0.4762	0.301	0.699	128371
Annular 91	75.68	109.67	185.35	0.0119	0.0189	0.4620	0.306	0.694	128371

Tables 4-11 and 4-12 show the pressure loss in the square and hexagonal lattices. The total mass flux in the core is constant while the share between inner and outer channels varies. The mass flux in the outer channels is proportional to the number of fuel elements, and negatively correlated with the inner channels. On the other hand, the friction coefficients, i.e. in inner channel, outer channel and at the spacer grid, correlate with the number of elements. The pressure drop characteristics are similar to those reported by Kazimi [93], which suffices to validate the model.

4.5 Conclusions

These calculations provide analytical solutions of the default (solid) and innovative (annular) fuel approaches. The temperature distributions in the “hot” fuel rod including cladding, gas gap and fuel together with pressure drops across the fuel channels were obtained. Seven new designs were prepared and estimated during the calculation process. For a given operating condition and modelling assumptions, the maximum temperature decreases with number of annular elements. The annular fuel is superior in case of maximum fuel temperature, which is up to 757°C lower than the reference design with the use of spacer grids. However, the pressure drop is proportional to number of fuel elements, but the optimal design that trades-off between temperature distribution and pressure drop is not yet determined. The pressure drop with spacer grids is usually smaller than the default design. This study suggests the most interesting designs are the

hexagonal lattice with 91 fuel elements and the square lattice of 18×18 where the maximum temperatures are 822°C and 732°C , while pressure drops of 185 kPa and 128 kPa, are observed respectively. In the case of the hexagonal lattice, the pressure drop is higher than in the default design while the square lattice is more promising due to the similar or lower pressure drop, i.e. 132 kPa, allowing for the use of a smaller pump.

These preliminary results show the annular fuel concept has the potential to increase both performance and safety, due to superior cooling capacity and in the case of square lattice, the pressure drop can be reduced if needed. Moreover, the square lattice allows the uprating of the power output to 110% of nominal power while meeting safety requirements, i.e. temperature and coolant velocity criteria, and is worth further development and evaluation. The hexagonal lattice, on the other hand, is characterized by higher coolant velocity that limits power uprating.

Chapter 5

Safety Analysis of Supercritical Water Reactors*

This chapter reviews SuperCritical Water-cooled Reactor (SCWR) concepts. The current Generation III/III+ nuclear reactors operate with a working fluid in subcritical conditions ($T_{pc} = 647\text{K}$, $p_{cr} = 22.064\text{ MPa}$). Because the source and sink temperature ratio limits power output, SCWRs can raise efficiency by 30% when operating at supercritical conditions. Therefore, SCWRs are a promising advanced nuclear system and one of the most interesting Generation IV nuclear reactor technologies, with the possibility of a direct upgrade from GenIII light water reactors (LWRs). However, conversion technologies must ensure safe operation during normal and accidental conditions. Therefore, the review of safety analysis includes different reactor designs and approaches.

*This section published substantially as reference: Rowinski et al. (2015). "Safety Analysis of Supercritical Water Reactors - A Review." Submitted to: Progress in Nuclear Energy

5.1 Introduction

SuperCritical Water-cooled Reactors (SCWRs) are an incremental evolution of the currently used Generation III/III+ light water reactors (LWRs), which will allow more efficient resource utilization. The Generation IV Forum (GIF) [15, 119] investigated six different reactor technologies, i.e. Very High Temperature Reactor (VHTR), Sodium-cooled Fast Reactor (SFR), Lead-cooled Fast Reactor (LFR), Gas-cooled Fast Reactor (GFR) and molten salt reactor (MSR), with SCWR being one of the most promising concepts. The goals advanced Generation IV (GenIV) reactors are improved sustainability, economics, safety and reliability together with proliferation resistance and physical protection. Sustainable energy generation includes meeting clean air objectives together with providing long term availability and effective utilization of fuel. Moreover, nuclear waste production should be minimized. GenIV reactors should also ensure financial risks and life-cycle cost are competitive with other energy sources. Moreover, ease of operation and maintenance should be ensured. The safety and reliability objectives state that the probability of severe accident must be $<10^{-5}$ accident per year. Another important feature is the ability to withstand a severe accident without offsite emergency response. Therefore, the reactor building must contain all contamination sources until emergency services take action. Finally, advanced reactors should be unattractive sources of weapon-usable material and offer physical protection against natural disasters and terrorism. As the SCWR is a direct evolution of LWRs, it can be treated as a combination of pressurized water reactor (PWR) and boiling water reactor (BWR). Within the SCWR pressure vessel (RPV), the working fluid does not change state as in a PWR, but rather the supercritical fluid/steam goes directly from RPV to the turbine as for BWR. Therefore, SCWRs need neither separate steam generators nor built-in RPV steam separators and dryers, which reduces complexity, size, and mass of the reactor and improves safety (fewer mechanical parts result in a lower chance of failure). Use of water above critical point ($T_{pc} = 647\text{K}$, $p_{cr} = 22.064\text{MPa}$) can improve LWR efficiency by up to 30%. Taken together, the characteristics of SCWR make the design a promising candidate for deployment in the near future.

This chapter presents the evaluations carried out by a number of countries to ensure the safety of the six most advanced SCWR designs, which have progressed to different stages.

5.2 Basis of Safety Analysis

The safety analysis should include fuel assembly design, emergency cooling systems, and response to transient and accidental conditions. Table 5-1 shows the most important information about different SCWR designs. The main difference between these concepts is the neutron spectrum. The thermal reactors require a moderator to slow the neutrons to maintain the fission reaction, whereas a fast reactor, such as SWFR, is moderated to ensure the blanket fuel absorbs neutrons instead of causing fast fission, and avoid negative void reactivity without complicating the core design. The Canadian SCWR is characterized by the highest operating temperature, hence, its efficiency is the highest.

Table 5-1 Summary of design parameters of different SCWR designs [120-127]

	Super LWR	SWFR	HPLWR	SSCWR	Canadian SCWR	SCWR-M	VVER-SCP	US SCWR	SCWR-SM
Origin	Japan		EU		Canada	China	Russia	USA	Korea
Neutron Spectrum	Thermal	Fast	Thermal	Thermal	Thermal	Mixed	Fast-resonance	Thermal	Thermal
Thermal Power	4 GW	1.6 GW	2.3 GW	2.4 GW	2.5 GW	3.8 GW	3.8 GW	3.6 GW	3.2 GW
Pressure	25 MPa	25 MPa	25 MPa	25 MPa	25 MPa	25 MPa	24.5 MPa	25 MPa	25 MPa
T_{in}	290°C	280°C	280°C	280°C	350°C	280°C	290°C	280°C	280°C
T_{out}	510°C	508°C	500°C	500°C	625°C	510°C	540°C	500°C	510°C
Moderator	H ₂ O	ZrH	H ₂ O	H ₂ O	D ₂ O	H ₂ O	H ₂ O	H ₂ O	ZrH ₂
No of Pass Through Core	Two-pass	Two-pass	Three-Pass	One-Pass	One-Pass	Two-pass	One-Pass and Two-Pass	One-Pass	One-Pass

From the safety and operational point of view the number of passes through the core influences coolant, moderator and fuel behavior. A one-pass core is a simpler design and provides natural circulation that improves safety. However, three concerns arise: (i) axial peaking factor is large, (ii) it is difficult to ensure a negative void reactivity coefficient at the end of fuel life cycle, and (iii) a huge increase in enthalpy along the channel may lead to overheating of fuel elements. Solutions to these problems require the use of different fuel enrichment in the axial direction and/or additional moderation in the upper part of the core. A multi-pass flow in the core avoids negative void reactivity coefficients throughout the fuel life cycle without special engineering, as between each pass the flow mixes to avoid hot fuel rod spots from the high rise of enthalpy. The drawback of this concept is high pressure loss that reduces the effectiveness of natural circulation.

5.2.1 Fuel design

Nuclear power plants (NPP) must be secured in any conditions during the operating lifetime including abnormal transient and accidental conditions. The first barrier to prevent radioactive material release is the fuel rod, which consists of fuel pellets, gas gap, and cladding as a part of the defence-in-depth approach [128]. Currently, zircalloy is a standard material for contemporary LWRs, however, it does not possess the required strength at supercritical water conditions, and must be replaced with different materials.

To this end, a Japanese research team [129] has investigated austenitic stainless steel 304 (SS304) and used the FEMAXI-6 fuel analysis code to evaluate the capability of this material to withstand overheating and overpower transients. The analysis was conducted for the Super LWR since at that time experimental data were unavailable to confirm the fuel integrity. The simulations conservatively assumed:

- (i) the pressure difference in the cladding should be less than 1/3 of the collapse pressure of the cladding;
- (ii) the strain on the cladding should not exceed the elastic limit (i.e., no plastic strain on the cladding);
- (iii) the fuel pellet centreline temperature should be less than its melting point;
- (iv) the system pressure should not exceed 28.9 MPa (105% of the maximum pressure for normal operation); and
- (v) the internal pressure of the fuel rod should not become excessively high (less than the coolant pressure during normal operation).

With the assumptions made during the evaluation and taking account of the behaviour of zircalloy under irradiation, the Maximum Cladding Surface Temperature (MCST) was estimated to be 950°C. Moreover, due to the lack of experimental results with stainless steel under similar conditions, an additional margin of 100°C was set. Thus, the proposed peak cladding temperature was estimated as 850°C during the transient conditions.

Currently, an experimental investigation of a 2×2 fuel assembly is ongoing in an LVR-15 research reactor in Rez, the Czech Republic, as a part of the “Supercritical Water Reactor – Fuel Qualification Test” (SCWR-FQT) program [130]. It is part of the European-Chinese cooperation through the project Supercritical water cooled IN-PILE

Test (SCRIPT), where the loop parameters can reach 600°C and 25 MPa. However, the temperature is lower than in tests conducted in autoclaves, i.e. 650°C, where it was stated that “Under the assumption that the conventional part of an HPLWR is operated at or below a maximum temperature/pressure of 650°C/25 MPa, one can conclude that, from a standpoint of creep-rupture strength, corrosion resistance and irradiation behaviour, not only Ni-alloys but also high-strength austenitic stainless steels can fulfil the requirements for *in-core cladding and structural materials*” [131]. On the other hand, the LOCA criteria estimate the maximum temperature as 1260°C since the SCWR first designs [132]. It is noted that the Minimum Deterioration Heat Flux Ratio (MDHFR) does not influence the design process as found by Kitoh et al. [133]. Therefore, only the cladding material performance is considered as a limit for the SCWR.

The SCWR-FQT started in 2011 with a duration of about 48 months. The objectives are related to the design, analysis and licensing of the fuel assembly suitable for use in supercritical water conditions. Specifically, these are:

- (i) to design a test section, a supercritical water loop and all safety and auxiliary systems required for safe operation of such a fuel assembly test;
- (ii) to analyse the test equipment under normal and accidental conditions to demonstrate safe operation;
- (iii) to build and operate with supercritical water an out-of-pile test assembly having the same test section geometry, but heated electrically;
- (iv) to validate codes for thermal-hydraulic predictions of the flow structure in SCWR fuel assemblies, using the above mentioned out-of-pile test results;
- (v) to focus the material research on those in-core materials which could be licensed in the near future and to prepare a qualified, reliable material database;
- (vi) to complete the required licensing documentation for the fuel qualification test and establish if a nuclear facility operating at supercritical pressure can be licensed or, otherwise, to identify challenges associated with it; and
- (vii) to teach and train young scientists in licensing procedures of nuclear facilities including the required quality management methods.

Figure 5-1 shows the details of the design of the test section inside the pressure tube. The tube contains four fuel rods that are filled with ^{235}U enriched to 19.7% and power of 64 kW.

Fig. 5-1 Design details of the test section inside the pressure tube (left) and the cross-section of the test section with the fuel assembly (right). Navy blue - U-tube cooler, light blue - recuperator tubes, pink - emergency cooling line, green - outer guide tube and yellow colour - inner guide tube. [130]

Table 5-2 shows the main parameters of the fuel assembly and operating conditions. The rod diameter is 8 mm while the pitch between fuel elements is 9.44 mm. Tests were conducted above the critical point of water, i.e. at 25 MPa pressure in order to gather information about the behaviour during the transition from sub- to supercritical temperatures.

Table 5-2 Parameters of fuel assembly and operating conditions [130]

Parameter	Value
Rod diameter (4 rods)	8 mm
Pitch	9.44 mm
Total rod height	709 mm
Fuel height	600 mm
Fissile power	63.6 kW
γ -heat power	9.8 kW
Nominal operating pressure	25 MPa
Nominal operating temperature at inlet of active channel	300°C
Nominal operating temperature at outlet active channel	300°C
Temperature of water in the test section (around fuel)	385°C
Nominal flow rate in active channel	900 kg/h
Total volume of water in primary circuit	57 dm ³
Coolant velocity around fuel rods	3-4 m/s

The full list of work packages of SCWR-FQT were as follows:

- (i) Design of the facility together with a test loop and necessary auxiliary systems. It must be done within constraints of the research reactor LVR-15;
- (ii) Analyses of normal operation including start-up and shut-down of the system, followed by detailed Computational Fluid Dynamics (CFD) analysis;
- (iii) Safety analyses of the defence in depth approach [134], to ensure fuel integrity during overheating and overpower events;
- (iv) Pre-qualification and selection of nuclear grade stainless steels tested in autoclaves and construction of similar test sections evaluated by electric heat rather than nuclear fuel irradiation;
- (v) Education and training of young scientists and students in workshops that involve analyses of SCWR; and
- (vi) Management, procedures and protocols.

5.2.2 Safety analysis

The safety analyses were conducted to ensure appropriate safety responses of the plant during normal operating and transient conditions. They can be divided into two parts, i.e. deterministic safety analysis and Probabilistic Safety Analysis (PSA), that provide assurance that all barriers can retain reactor integrity and prevent radioactive material release to the environment as far as possible in the event of an accident.

5.2.2.1 Deterministic safety analysis

This approach studies plant behaviour during operation and transient conditions should a Postulated Initial Event (PIE) occur (Table 5-3). The possible occurrences are grouped to perform analysis of those resulting in severe accidents in terms of neutronic, thermohydraulic, radiological, thermomechanical and structural aspects with different computational tools. The codes incorporate a variety of conditions together with postulated Design Basis Accidents (DBAs) and evaluate the plant response using an adequate set of conservative or best estimate assumptions for the initial and boundary conditions. A successful design will shut down the NPP while the residual heat is removed from the reactor core. Moreover, radioactive release must be minimized or below regulatory limits. The evaluation period must be long enough to ensure that the NPP has reached stable and safe shut down conditions.

Table 5-3 Possible subdivision of postulated initiating events [135]

Occurrence (1/reactor year)	Characteristics	Plant state	Terminology	Acceptance criteria
10^{-2}-1 (expected over the lifetime of the plant)	Expected	Anticipated operational occurrences	Anticipated transients, transients, frequent faults, incidents of more frequency, upset conditions, abnormal conditions	No additional fuel damage
10^{-4}-10^{-2} (chance greater than 1% over the lifetime of the plant)	Possible	Design basis accidents	Infrequent incidents, infrequent faults, limiting faults, emergency conditions	No radiological impact outside the exclusion zone
10^{-6}-10^{-4} (chances less than 1% over the lifetime of the plant)	Unlikely	Beyond basis accidents	Faulted conditions	Radiological consequences outside the exclusion area within limits
$<10^{-6}$ (very unlikely to occur)	Remote	Severe accidents	Faulted conditions	Emergency response needed

The deterministic analysis is conducted using conservative assumptions to ensure the reliability of the systems during operation or transient conditions, and all limits must include safety margins. In accidents, the evaluation should be realistic and develop adequate emergency procedures with realistic initial and boundary conditions. To estimate uncertainty, the conditions are combined statistically. Hence, in the deterministic analysis, the conservative and best estimate approach is used.

5.2.2.2 Probability safety analysis (PSA)

The PSA, uses a probabilistic approach to predict the core damage frequency (CDF), societal or individual risks, and susceptible design features of the NPP. The analysis recognizes the vulnerable points of the plant by forcing designers to perform a complete examination of possible event sequences without excluding less severe PIE as the deterministic approach does. Therefore, PSA can be used for Level 1 or Level 2 events [136, 137] that may lead to CDF and the release of radioactive material.

The analysis develops event trees connecting transients, accidents or other events with a probability of a plant failure. Therefore, plant vulnerabilities can be predicted together with operational weaknesses that cannot be predicted using a deterministic approach. An early, simplified PSA of SCWR was conducted by Lee et al. in 1999 [138], while one of the first PSA in the world was the report NUREG-1150 [139].

5.2.3 The Safety Systems of SCWRs

The safety analysis criteria can be divided into three categories, i.e. normal operation, abnormal transient and accident conditions. During normal operation SCWR does not behave as other water cooled reactors having neither a recirculation loop nor primary circuit like BWR or PWR (Fig. 5-2). The supercritical fluid flows to the turbine straight from the Reactor Pressure Vessel (RPV) separators or dryers as safety features.

Since at supercritical conditions it is impossible to differentiate the fluid and gas phases, control of water level as in other LWRs is unavailable. Therefore, the safety principle of the SCWR is to maintain the coolant flow in the reactor core, by monitoring the RPV inlet pumps and outlet valves (Table 5-4).

Fig. 5-2 Comparison of plant systems [140]

Table 5-4 Comparison of safety principles in water cooled reactors

	PWR	BWR	SCWR
Requirement	Primary coolant inventory	Coolant inventory in the reactor vessel	Coolant flow rate in the core
Monitored parameter	Water level in the pressurizer	Water level in the reactor vessel	Main coolant flow rate, turbine inlet pressure

Figure 5-3 shows a typical safety system deployment in SCWR known as the Emergency Core Cooling System (ECCS), the main parts being:

- (i) containment,
- (ii) Main Steam Isolation Valves (MSIVs),
- (iii) Automatic Depressurization System (ADS),
- (iv) Auxiliary Feedwater System (AFS),
- (v) Low Pressure Core Injection (LPCI) system, and
- (vi) suppression chamber.

Fig. 5-3 Safety system deployment [141]

5.3 Safety Analysis

Safety analysis is the crucial part of the design process. According to many research papers, the safety approach should secure the maximum cladding surface temperature (MCST) to below 850°C during abnormal transient conditions [129] and 1260 °C in case of accidents that may lead to core damage [142], to avoid severe environmental repercussions. These criteria are conservative, and small excesses should not lead to radioactive material leakage.

Since SCWR technology is neither matured nor licensed, lessons must be learned from similar reactor types. A commonly used practice is to conduct Computational Fluid Dynamics for early designs and then conduct experiments to validate the results. CFD allows researchers to perform detailed analysis of the system. Because SCWR is less developed, detailed reviews such as '*CFD4NRS with a focus on experimental and CMFD investigations of bubbly flow*' that contains current trends related to reactor safety have not been conducted [143]. A key information source for performing CFD simulations for Nuclear Reactor Safety (NRS) is released by the Nuclear Energy Agency (NEA) is the '*Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Application*' [144]. In 2014, a Special Issue of the 4th Workshop on the CFD for Nuclear Reactor Safety (CFD4NRS-4) [145] was released. It reviewed papers related to NRS and the proper conduct of CFD analysis valid for design applications. The main conclusion was that the Best Practice Guidelines are "almost universal" in conducting CFD simulations but a balance is required for sensitivity studies that can be computationally intensive.

5.3.1 Japanese Approach

Japan is the only country that is pursuing two designs simultaneously. The first is the Supercritical Light Water cooled Reactor (Super LWR) that operates with a moderator in the form of so-called water rods inside the fuel assemblies. The water rods consist of a space filled with light water under subcritical conditions to moderate neutrons and to secure a negative void reactivity coefficient. Second, a fast neutron spectrum reactor is under development and where zirconium-hydride layers ensure a negative void coefficient. Therefore, these two concepts will be presented together to evaluate the different behaviours.

Both concepts have been investigated since the early 90's and are the most advanced SCWR designs, with the outlet temperature rising from 410°C to 500°C and efficiency from 40% to 44%, due to improved materials science. Oka et al. [132] summarized the characteristics of the thermal-neutron-spectrum reactor (SCLWR), fast breeder reactor (SCFBR-D) and fast converter reactor (SCFR-D) and reported average outlet temperatures of 407-431°C and efficiencies of 40.7 – 41.5%. Currently, the SCWRs have an efficiency of about 44% and an average outlet temperature of up to 530°C [127, 140].

In order to conduct safety evaluations of both SCWRs, sub-channel codes that can handle subcritical fluids and supercritical-subcritical transitions were developed. The first attempt to evaluate the development of LOCA in SCWR was the SCRELA code [146]. All of the codes use point kinetics for neurotic calculations (Table 5-5).

Table 5-5 Codes for Safety analysis of Super LWR [147]

Code	Initial conditions	Analyzed event
SPRAT-DOWN	Stead-state at supercritical conditions	Abnormal transients or accidents, including small LOCA without depressurization
SPRAT-DOWN-SUB	Stead-state at subcritical conditions	Abnormal transients or accidents
SPRAT-DOWN-DP	Stead-state at subcritical conditions	Blowdown at large LOCA or reactor depressurization
SCRELA reflood module	End stage of blowdown	Core reflooding after blowdown

Figure 5-4 shows an example of the flow chart for the SPRAT-DOWN sub-channel code, that is similar to other commonly used codes to perform analyses of LWRs, that sets initial conditions and evaluates the inlet parameters such as flow rate and temperature. Next, mass and energy conservations are obtained to proceed with the calculation of pressure drops in the channels and the evaluation of momentum and flow balances at the

outlet. If the pressure drop in the average and hottest channels are balanced, the heat exchange between coolant and fuel rods is calculated. This is valid for all time steps.

Fig. 5-4 Flow chart of transient analysis on the SWFR [148]

Figure 5-5 presents an example of the SPRAT-DOWN model for safety analyses of the Super LWR, which can be applied to any kind of SCWR including fast reactors. At the beginning of calculations, the flow fractions entering the upper dome and the lower plenum must be specified. Then, the flows are directed to either the average or hot

channels, followed by the calculation procedure described earlier. All of the safety systems such as MSIV, AFS etc. are taken into account and their parameters are implemented into the codes.

For both approaches, i.e. Super LWR and SWFR, ten abnormal transients were investigated during the safety analysis with the main assumptions being:

- (i) *Partial loss of reactor coolant flow* – only one of the feedwater pump is offline.
- (ii) *Loss of offsite power* – motor driven condensate pump trips.
- (iii) *Loss of turbine load* – all main steam isolation valves (MSIVs) are closed or open.
- (iv) *Isolation of main steam line* – the same as previous cases without turbine bypass.
- (v) *Pressure control system failure* – maximum turbine control valve is open at 130% rated value.
- (vi) *Loss of feedwater heating* – loss of one stage feedwater heater, hence the inlet feedwater temperature is assumed to decrease from 280°C to 225°C.
- (vii) *Inadvertent start-up of AFS* – all auxiliary systems are on and thus 12% rated value coolant flow enters the core at 30°C.
- (viii) *Reactor coolant flow control system failure* – feedwater pumps supply 138% of nominal flow.
- (ix) *Uncontrolled CR withdrawal at normal operation* – the rod reactivity is 1.05% dk/k at a withdrawal speed of 1.14 m/min leading to inserted reactivity of 0.69%.
- (x) *Uncontrolled CR withdrawal at start-up* – the rod's reactivity is 2.8% dk/k and coolant temperature of 280°C at a withdrawal speed of 1.14 m/min leading to inserted reactivity of 0.39%.

The safety analysis also contains accident evaluations including DBA, such as:

- (i) Total loss of feedwater flow;
- (ii) Reactor coolant pump seizure;
- (iii) Control rod ejection (hot standby); and
- (iv) Control rod ejection (operation).

Since the reactor scrams when the feedwater flow decreases to 90%, or if the operating pressure change is higher or lower than the Level 1 limit, the first signal of abnormal operation always triggers a scram (Table 5-6). A summary of the safety design in Super LWR can be found in Table 5-7.

Fig. 5-5 Calculation model of SPRAT-DOWN for safety analyses [147]

Table 5-6 Principle of system safety actuation [149]

Flow rate low (feedwater or main steam)	
Level 1 (90%)	Reactor scram
Level 2 (20%)	AFS
Level 3 (6%)	ADS/LPCI system
Pressure high	
Level 1 (26.0 MPa)	Reactor scram
Level 2 (26.2 MPa)	SRV

Pressure low	
Level 1 (24.0 MPa)	Reactor scram
Level 2 (23.5 MPa)	ADS/LPCI system

From Table 5-7 shows those systems that will be switched on during abnormal operation. It is worth mentioning that the “2-out-of-4” logic for independent detectors is used. Most of the scram signals are taken from either PWR, BWR or both designs. Nevertheless, since the main coolant flow rate is the most important for the Super LWR, specific signals for SCWR are also introduced as scram signals are not required in other reactor technologies. These signals are: condensate pump trip, loss of offsite power and turbine control valve closure. The reactor coolant pump trip itself is retained as a scram signal.

Table 5-7 Summary of safety system design [147]

Safety system	Actuation conditions				
Reactor scram system	Pressure high (level 1)			Main coolant flow rate low (level 1)	
	Pressure low (level 1)			Reactor power high (120%)	
	MSIV closure (90%)			Turbine control valve quickly closed	
	ECCS start-up			Main stop valve closure	
	Drywell pressure high			Earthquake acceleration large	
	Reactor period short (10s)			Loss of offsite power	
	Reactor coolant pump			Condensate pump trip	
AFS (4% capacity x 3 units) (Turbine-driven)	Reactor coolant pump trip			Main coolant flow rate low (level 2)	
	Loss of offsite power			Turbine control valves quickly closed	
	Condensate pump trip			Main stop valves closure MSIV closure (90%)	
SRV (20% capacity x 8 units)	Relief valve function			Safety valve function	
	Open	Close	Number	Open	Number
	(MPa)	(MPa)		(MPa)	
	26.2	25.2	1	27.0	2
	26.4	25.4	1	27.2	3
	26.6	25.6	3	27.4	3
ADS (20% capacity x 8 units) MSIV	Pressure low (level 2)				
	Main coolant flow rate low (level 3)				
LPCI (12% capacity x 3 units) (Motor-driven)	Drywell pressure high				

5.3.1.1 Supercritical light water cooled reactor (Super LWR)

The first attempt to design a SCWR using thermal neutrons with water rod moderation dates back to 1994 by Okano et al. [120] where in 1997 a safety analysis of the early design of Super LWR [149] was conducted using the SPRAT code. It was concluded that Super LWR satisfied all safety criteria at that time.

The Super LWR emergency core cooling system (ECCS) consisted of an auxiliary feedwater system (AFS), low pressure injection system (LPCI), automatic depressurization system (ADS) and main steam isolation valves (MSIVs), and was adapted from an Advanced Boiling Water Reactor (ABWR). Figure 5-6 shows the coolant flow pattern during depressurization, i.e. the MSIV are closed and the ADS directs the coolant into a suppression chamber, while the coolant is injected by feedwater pumps to the LPCI.

Fig. 5-6 Coolant flow during depressurization [150]

5.3.1.1.1 Abnormal transients

A list of abnormal transients was presented earlier, but as only some cause an increase of the pressure or temperature, not every event is presented in the following estimation. The criteria of safety margins for transients were set at 850°C and 28.875 MPa.

Fig. 5-7 Summary of increases in hottest cladding temperature at abnormal transients (criteria 850°C) [147]

Figure 5-7 shows the temperature increase during abnormal transients with a substantial margin for safety. As expected, the partial loss of reactor coolant flow is the most dangerous transient, but well below the postulated temperature limit for the cladding material.

Figure 5-8 shows the peak pressure in the reactor during abnormal transients where the case of all main steam isolation valves (MSIVs) closed proving most severe. Knowing that the operating pressure is 25 MPa, the other cases barely influence the reactor vessel pressure.

Fig. 5-8 Summary of peak pressures at abnormal transients (criteria 28.875 MPa) [147]

Fig. 5-9 Summary of increases in hottest cladding temperature during ATWS (criteria 1260°C) [151]

Fig. 5-10 Summary of peak pressures during ATWS (criteria 30.25 MPa) [151]

5.3.1.1.2 Anticipated transients without scram (ATWS)

The ATWS events might be dangerous if the reactor continues working. Therefore, the reactor should behave safely and without damage to the cladding barrier throughout. Figure 5-9 presents the increase of cladding surface temperature in the “hot” fuel rod, and shows three events that lead to the same maximum temperature increase in the case of ATWS without alternative action, i.e. (i) loss of offsite power, (ii) loss of turbine load, and (iii) isolation of the main steam line. In the first event, the motor driven condensate pump trips, whereas in the other two, the MSIV are closed. Nevertheless, in all events, the temperatures are at least 100°C below the safety limit of 1260°C. In all cases, the temperatures would be higher without a safety response. The highest pressure peak occurs during the loss of turbine load, no matter if action is taken. In the case of isolation of the main steam line, the pressure peak is higher with alternative action (Fig. 5-10).

5.3.1.1.3 Accidents and PSA

In the case of safety analysis, the frequencies of initiating events used for Probabilistic Safety Assessment (PSA) are taken either from PWR or BWR calculations. Since the reactor vessel is very similar to those in PWRs, the LOCAs frequencies are taken from PWRs. In the case of abnormal transients, the frequencies are taken from BWRs. Hence, it is possible to estimate core damage frequency for the Super LWR. Figure 5-11 shows that large LOCA may be the most severe accident and have the greatest share in CDF events. The sum of all CDF events is estimated to be approximately 10^{-6} per year [147]. It can be seen that even in conceptual designs, it was possible to conduct satisfactory PSA. Further decrease of CDF is possible if the analysis includes an auxiliary feedwater system (AFS) and automatic depressurization system (ADS) optimized for SCWRs.

Fig. 5-11 CDF from each initiating event [147]: LOCA – Loss of Coolant Accident, LOSP – Loss of Offsite Power, T-PCS – Transients with Power Conversion System (PCS) available at the initial stage, T-nPCS – Transients with PCS unavailable at the initial stage.

5.3.1.2 Supercritical water cooled fast reactor (SWFR)

Since SWFR is in development by the same institution as Super LWR, the safety systems are similar, the main difference being the lack of water rods inside the RPV core. After the first fast breeder reactor conceptual design cooled by supercritical steam in 1992 and 1993 by Oka et al. and Jevremovic et al. [152, 153], it was proposed in 1993 by

Jevremovic et al. [154] to use zirconium-hydrate ($\text{ZrH}_{1.7}$) to ensure a negative void reactivity coefficient. In 1996, $\text{ZrH}_{1.7}$ was evaluated by Oka et al. [155] to be sufficient for this purpose. While the design has evolved, safety analyses can be found at every stage, the most recent by Sutano and Oka [156] in 2014. All of the safety analyses were performed using specialised codes as presented in Table 5-4. The safety analyses were performed in previous years by Ikejiri et al. and Li et al. in 2010 and 2013 [141, 157].

5.3.1.2.1 Abnormal transients

A compilation of investigated abnormal transients is shown in section 5.3.1. The maximum cladding surface temperature (MCST) is presented in figure 5-12, together with evaluations at both Beginning of Life (BOL) and End of Life (EOL) stages. The criteria for the temperature and pressure during transients are 850°C and 28.875 MPa, respectively, the same as for Super LWR. Usually, the temperature is higher at the EOL during abnormal transients. Nevertheless, the highest MCST occurs at BOL during pressure control system failure, i.e. the turbine control valve is open at 130% of normal flow, thus less medium is cooling the fuel rods, but all temperatures are below the criteria of the cladding material by more than 100°C.

In the case of the peak pressure during the abnormal transients (Fig. 5-13), there are negligible differences between values at BOL and EOL. In the first case, the pressure is slightly higher in some of the events. All of the values are within safety criteria and well below critical limits. The highest pressure occurs during isolation of the main steam line when all MSIVs are closed and steam is unable to escape the RPV.

5.3.1.2.2 Accidents

Accidents are evaluated with the same codes as abnormal transients. BOL and EOL were studied and a list of evaluated events can be found in section 5.3.1. The criteria for the temperature and pressure are 1260°C and 30.25 MPa, respectively.

Fig. 5-12 Summary of increases in hottest cladding temperature at abnormal transients (criteria 850°C) [156]

Fig. 5-13 Summary of peak pressures at abnormal transients (criteria 28.875 MPa) [156]

Figure 5-14 shows the prediction of MCST during accident conditions. The highest MCST is predicted at EOL during control rod ejection at operating conditions, i.e. 899°C, is more than 360°C below the safety limit for accident conditions and only 49°C above the conservative criteria for abnormal transient conditions. The smallest impact on the increase of the MCST has rod ejection during standby since the accident starts at relatively low temperature.

Fig. 5-14 Summary of increases in hottest cladding temperature during accidents (criteria 1260°C) [156]

On the other hand, the pressure distribution during an accident conditions (Fig. 5-15) shows that rod ejection at standby conditions has the largest values, both at BOL and EOL. The maximum peak pressure is 28 MPa at EOL. LOCA accidents do not have much influence on the pressure since line breaks generally decrease pressure.

Fig. 5-15 Summary of peak pressures during accidents (criteria 30.25 MPa) [156]

5.3.2 European Approach – HPLWR

The European HPLWR is a three-pass core consisting of an evaporator and two superheaters, that limits the reactor height. On the other hand, uniform mixing in the lower and upper plenums is necessary to avoid generation of overheated spots in the fuel assemblies. Numerous work has been done in order to predict the occurrence of the HTD phenomenon with CFD calculations has been undertaken. Palko and Anglart stated that the $k-\omega$ SST turbulent model gives the most accurate prediction of HTD events [158].

Although HPLWR is based on the Japanese designs, none of the codes listed in Table 5-4 were used to conduct a safety analysis of the reactor. The most reliable codes including RELAP5, TRAB, and CATHARE are ongoing modifications to evaluate supercritical systems [103], while China is developing a Subchannel Analysis Code of SCWR (SACoS) that was benchmarked against HPLWR calculations [159]. In the case of neutronic calculations, HPLWR uses MCNPX and HELIOS-2, where it was concluded that “although MCNPX is better HELIOS-2 is faster” [160]. Schulenberg presented a design and analysis of the thermal core of HPLWR that has sufficient margins for MCST during operation and the wire wrapped fuel rods can improve the mixing of the coolant preventing HTD. However, the individual fuel rod peaks due to different burnup, control rods position, etc. are not yet evaluated [161]. The use of wire wrapped fuel rods to improve the mixing of the supercritical fluid was also evaluated by Schulenberg [162]. To this point, the analyses were conducted to achieve safety requirements during operating conditions. Subsequently, codes must be validated with the test loop described in section 5.2.1. Figure 5-16 shows the scheme of the fuel qualification test loop (FQT) that is used to research SCWR.

3.3.2.1 Simplified Supercritical Water Reactor (SSCWR)

The Simplified SuperCritical Water-cooled Reactor (SSCWR) is based on HPLWR with similar performance and a once through core with a number of mixing zones. Currently, the analysis is limited to ensure an average outlet temperature of 500°C. The design proposed by Reiss evolved from a core with 3 heating zones [163] to a core with 6 different heating zones which also increased the height of the core to 6 meters [104]. Further evaluation is necessary, as the relatively high active fuel zone may cause xenon oscillations.

Fig. 5-16 Schematic illustration of the FQT loop [164]

5.3.3 Canadian Approach – CANDU-SCWR

The Canadian Atomic Energy of Canada Limited (AECL) is cooperating with China to develop a CANDU-SCWR, and China is preparing and validating a subchannel code SUBCHAN. During its development, the code was validated under subcritical conditions against the ASSERT-PV code initially, then afterwards at supercritical pressure, i.e. 25 MPa. The wall temperature distribution evaluated by the SUBCHAN code showed two peaks; the first is rather narrow at 0.5m from the inlet due to the decrease of heat transfer coefficient while the temperature crosses the critical point, i.e. the heat transfer deterioration (HTD) effect, whereas the second one is much wider and is the natural result of a constant increase of coolant temperature [165].

The newest calculations by Li et al. in 2009 does not show HTD because the fuel rods configuration was optimized [122]. Similar behaviour was found by Yu et al. [166]. Therefore, it can be concluded that the wall temperature during normal operation

increases steadily with peak temperature of around 800°C. Those calculations were conducted with subchannel codes “ATHAS” and SUBCHAN, respectively.

Numerous work has been done with the use of numerical methods to optimize the fuel assembly design or material, e.g. use of Yttria Stabilized Zirconia (YSZ) as a ceramic insulator inside pressure tubes [167]. The optimization of the whole system cycle focusing on efficiency management and possible fuel material in the reactor was done by Naidin et al. [168]. Fluid-to-fluid scaling has been widely studied due to the ease of building test loops that use working fluids with lower parameters to achieve a supercritical phase [169, 170]. Comprehensive surveys were prepared by Pioro and Duffey from 2004-2005 in order to collect experimental data concerning the use of supercritical water [171], empirical correlations of heat transfer in supercritical conditions [172] and to review the performance of supercritical carbon dioxide [173]. It was concluded that HTD can be predicted accurately, however, a universal correlation for heat transfer was not possible. Podila et al. conducted numerous CFD investigations on Canadian SCWR with and without wire wraps, and concluded that the $k-\varepsilon$ SST turbulent model can predict HTD phenomenon when $y^+ < 1$, whereas the RSM model is unable to do so. Moreover, the wire wraps increase secondary flow mixing, leading to lower wall temperatures [174, 175].

5.3.4 Chinese Approach

The Chinese mixed spectrum neutron reactor is unique. The two-pass core with fast spectrum at the centre and thermal spectrum in the outer parts of the reactor proves more challenging when conducting safety analyses that emphasize maintaining the cladding temperature below acceptable limits. Only two of the most severe accidents were evaluated, the Loss Of Flow Accident (LOFA) by Xu et al. and Zhu et al. [176, 177] and LOCA by Liu et al. [121].

The LOFA scenario was evaluated first by a modified RELAP5, where a thermo-physical package including supercritical water properties was implemented to perform the calculations by Xu et al. [176]. Secondly, Zhu et al. [177] developed TACOS (Transient Analysis Code Of SCWR). Both analyses show that the maximum cladding temperature is well below the acceptable limit, thus this accident will not compromise the integrity of the NPP. Moreover, a sensitivity analysis concluded that for SCWR-M, the maximum

cladding surface temperature (MCST) strongly depends on two factors: (i) pump coastdown time, where MCST decreases with it, and (ii) the AFS flow.

Evaluation of LOCA carried out by Liu et al. [121] was divided into two analyses, i.e. for the hot and cold leg LOCAs. It was found that the cold leg LOCA could be much more severe, and the safety system had to be reconsidered as the MCST rises close to 1600°C for a 25% break, which greatly exceeds the safety criteria. However, this problem was solved with the addition of a second ADS unit and maintaining the MCST decreased to below 1200°C. Therefore, it can be concluded that the SCWR-M after modifications can withstand conditions during LOFA and LOCA.

Fig. 5-17 Outline of SCWR-M safety system [121]

Figure 5-17 presents an outline of the SCWR-M safety systems. It is more complex than the Japanese approach shown in Fig. 5-3, and consists of suppression pools, two Isolated Cooling Systems (ICS), two accumulators (ACC), two Gravity Driven Cooling Systems (GDCS) and four-stage Automatic Depressurization Systems (ADS). The Standby Liquid

Control System (SLCS) is provided for backup shutdown and Passive Containment Cooling System (PCCS).

The final design is not concluded as optimization of the fuel assembly and fuel management are ongoing. One of the proposed designs use an annular fuel where moderator flows inside the fuel rod and are insulated from heat generated inside the fuel rod, whereas the coolant flows in coolant channels between the rods. Investigation of different enrichment zones was conducted together with an evaluation of annular fuel by Zhao et al. [178]. Extensive work was done by Chen et al. [179] and Zang et al. [180] to find a more accurate formula for heat transfer correlation or to extend the subcritical correlation to be valid in supercritical region, respectively.

5.3.5 Russian Approach

The Russian Federation has investigated both one- and two-pass flow designs, and studied only reactor that uses resonance neutron spectrum. The country has over 15 000 reactor years of experience with various reactor types such as VVERs, PWRs, BWRs, and RBMKs [123]. Currently, it is trying to choose which technology would provide the best trade-off between safety, economy and efficiency. Specifically, the number of flow passes through the core is important from the safety perspective.

A test reactor facility of thermal power of 30 MW has been proposed to check all systems in a real environment [181], particularly, the evaluation of different fuel types under supercritical conditions. Moreover, a literature review with a number of heat transfer databases at supercritical pressure was prepared to collate data for heat transfer evaluation during the design process [182].

Figure 5-18 shows the sketch of a single-circuit RP inside the VVER-SCP containment, where safety systems include:

- (i) Main Steam Isolation Valves (MSIVs);
- (ii) a Passive Residual Heat Removal System from the core (PHRS);
- (iii) an emergency core cooling system and reactor makeup (PCFS accumulators and tanks, ECCS pumps);
- (iv) prevention of pressure increase in the containment (PPDS, spray system); and
- (v) heat removal from the containment (CECS).

Fig. 5-18 VVER-SCP safety systems [183]

5.4.6 United States of America Approach

Currently, USA has suspended the SCWR design program of a one-pass core reactor, but the design had evolved over several years. The first step in design and safety analysis was to adjust RELAP5-3D to include supercritical water properties in 2003 [184]. In the same year, a safety analysis by Davis et al. [185] found the thermal limits for cladding maximum temperatures in SCWR are 1260°C in the case of an accident and 840°C for transients. All researchers classified the repercussions of loss-of-feedwater as an accident “which is consistent with the classification of the complete loss-of-flow event in pressurized water reactors” [185]. However, it was uncertain if the U. S. Nuclear Regulatory commission will also classify loss-of-feedwater as an accident, hence, they are used for calculations of thermal limits as for the transients.

The first conclusion for the SCWR analysis was that distinct correlations of heat transfer can lead to completely different results. For example, the maximum cladding temperature is directly proportional to power when the Bishop correlation was used, but was inversely proportional to power for the Koshizuka-Oka correlation. Moreover, the reactor evaluation for the solid $\text{ZrH}_{1.6}$ moderator was found to satisfy the thermal limits of 840°C should a 50% reduction of feedwater occur. Total loss-of-feedwater is more challenging. If the coastdown of the main feedwater is 5s, the auxiliary feedwater systems have to supply at least 15% of the initial feedwater flow. However, a fast-opening, 100% capacity turbine bypass would reduce the maximum cladding temperature significantly. When the calculations were repeated with water rods rather than $\text{ZrH}_{1.6}$, higher safety margins result.

Fig. 5-19 Sketch of proposed passive cooling systems [186]

Subsequently, more challenges were discovered, including the maximum temperature of claddings exceeded thermal limits during steady state, that requires additional insulation of the water rods [124]. During loss-of-feedwater, the response time for the auxiliary feedwater system must be extremely fast, and much faster than for current PWRs.

Therefore, an innovative passive cooling system was developed and evaluated. This concept proposes additional feedwater tanks be connected to both hot and cold water legs to allow circulation during a loss-of-feedwater accident (Figure 5-19). A safety evaluation with RELAP5-3D showed satisfactory results, with all cases including short- and long-term loss-of-flow and LOCAs accidents initiated by large breaks in hot leg, cold leg, and steam line resulted in temperatures and pressures within safety limits [186].

5.5.7 Korean Approach

The Korean approach is unique due to the use of one-pass core with an internal flow recirculation and solid moderator in a form of ZrH_2 . It is based on the early design of Japanese Super LWR. The internal recirculation is done by jet pumps that are installed in the downcomer, thanks to this design, the coolant recirculates inside the reactor, hence the enthalpy rise is lower and maximum cladding temperature is within safety limits.

The Korean team has developed a transient safety analysis code TASS/SCWR that is based on TASS/SMR [187, 188]. The calculations were performed for Japanese Super LWR to see if the use of passive residual heat removal (PRHR) is able to handle two accidental conditions, i.e. total loss of feedwater and loss of load. It was concluded that the PRHR system successfully removed residual heat and limits for cladding temperature and pressure in RPV were within safety limits [125].

The test facility, named SPHINX (Supercritical Pressure Heat transfer Investigation for NeXt generation) was built and used to perform the test with supercritical CO_2 . The test loop is designed to perform single tube, single rod and rod bundle experiments at the range of pressure of 7.3 - 10.0 MPa [189]. Currently, the test loop performed heat transfer experiments with a single tube in an upward and downward direction to compare obtained results with heat transfer formulae, and the results deviate by around 20% with the measured data [190, 191].

5.4 Conclusions

The ongoing research in SCWR technology shows promising results. Among the research teams around the world, the Japanese designs from the University of Tokyo and Waseda University are the most advanced in terms of the whole system design. From the safety point of view, they have conducted full analysis at operating, transient and

accidental conditions. Both Super LWR and SCFR had proven their ability to ensure the safety of the reactor at any conditions. The core damage frequency is below the required maximum. European HPLWR is currently at the design stage and the analyses were limited to ensure safety at normal operating conditions. However, numerous experimental work with the use of test loops and other activities are currently in development. The Canadian designs of CANDU-SCWR and SSCWR were investigated in order to secure the required averaged outlet temperature and MCST are within the safety limits during normal operation. Numerical investigations were conducted to optimize the fuel assembly. The Chinese SCWR-M has evaluated the safety of LOCA and LOFA during operational conditions, and found the design required modifications such as additional ADS unit together with an increase of AFS flow. Numerous test loop experiments were made to optimize the fuel assembly. The Russian Federation has designed two reactors with one- and two-pass core flows to evaluate which gives the optimal trade-off between safety, economics and performance. The USA has suspended the SCWR program, however, the preliminary results were promising and ensured the safety of the reactor design. The Korean design is still in early design and safety analyses results are limited.

Chapter 6

Numerical Investigation of Supercritical Flow of CO₂ in a Vertical Tube*

The study of the supercritical fluids is crucial for advanced Generation IV nuclear reactors where carbon dioxide and water may be deployed. Since fuel element heat flux varies axially, it is imperative to understand the influence of a non-uniform flux in this direction. The literature provides experimental results only when a uniform heat flux is applied, whereas non-uniform heat fluxes are a more realistic thermal response for different stages of fuel burnup. Hence, simulations should reflect flow behaviour from the beginning of the fuel cycle, when a cosine distribution is observed, to the end of the cycle, when the peaking factor is skewed to the bottom of the fuel element. The numerical investigation was performed for a 2-D axisymmetric tube model tube with a Computational Fluid Dynamics (CFD) code. Non-uniform heat flux is represented by a 2-parameter equation describing variation along the axial direction to provide information about the heat transfer coefficient and heat transfer deterioration (HTD) in supercritical conditions and the key parameters influencing these factors. With a better understanding of HTD fuel elements overheating can be prevented.

*This section published substantially as reference: Rowinski et al. (2015). "Numerical Investigation of Supercritical Flow in a Vertical Tube under Non-Uniform Heat Flux", 23rd International Conference on Nuclear Engineering (ICONE), May 2015, Makuhari, Japan.

6.1 Introduction

Constant growth in population and energy demand requires better ways to provide energy more efficiently. Since one of the most useful forms of energy is electrical energy, a key need is to either build new, more advanced power stations or upgrade the current fleet of power plants. The current nuclear power plant (NPP) technology is approaching its efficiency limit of 38% due to the suboptimal use of coolant. Years ago, conventional thermal power plants overcame this limit by increasing the pressure and temperature of the working fluid (steam/water) above the critical point, and increase the efficiency to 45%. Currently, the aim is to develop thermal power plants using ultra-supercritical parameters, and to break the barrier of 50% efficiency.

The concepts of NPP operating at supercritical conditions have been investigated since the beginning of the nuclear era, even though at that time materials science was not sufficiently advanced to ensure robust operability in a highly radioactive environment. The Generation IV international forum (GIF) is examining numerous designs including Advanced Gas-cooled Reactors (AGRs), SuperCritical Water-cooled Reactors (SCWRs) and Liquid Metal-cooled Reactors (LMCRs) [119] of which LMCRs use supercritical fluid in the second loop and SCWRs as a primary coolant.

SuperCritical Water-cooled Reactor (SCWR) concepts have attracted renewed interest since material science has made significant progress, and conventional thermal power plants have used supercritical water for decades, that improves the feasibility of adopting this technology. In terms of building a supercritical test loop, supercritical carbon dioxide (CO₂) is a simpler working fluid compared to water. CO₂ has much lower critical point ($p_{cr} = 7.38$ MPa, $T_{cr} = 31.04^\circ\text{C}$) than water ($p_{cr} = 22.064$ MPa, $T_{cr} = 373.9^\circ\text{C}$). For both fluids, simulations at the pre-design evaluation were validated against experimental data where the boundary conditions were similar to the calculations.

6.2 Numerical Approach

Experimental investigations are expensive as they require building a facility able to perform either scaled or non-scaled experiments. Hence, the use of numerical methods is more convenient, and save significant costs since expensive data logging instrumentation are not needed. Therefore, computer analyses are much cheaper and more efficient, However, experiments should be conducted to verify the numerical results.

One of the most common ways to simulate real experiment is to use Computational Fluid Dynamics (CFD). It is a powerful tool that allows the user to predict accurately all of the phenomenon ongoing during the experiment with the use of a computer. Hence, many researchers perform calculations using commercial or self-developed CFD codes.

6.2.1 Heat Flux Distribution

Heat flux distribution along the axis of a fuel element is non-uniform, following a sinusoidal curve characterized by Blakeman as [192]:

$$q''(z) = \left[\sin \left(\pi \left(x / H \right)^{1/N1} \right) \right]^{N2} \quad (40)$$

where x is the axis distance, H the height, $N1$ the parameter that controls the height of heat flux peak, and $N2$ the parameter that controls the slope of heat flux.

By modifying parameters $N1$ and $N2$, the heat flux distribution can be adjusted as flatter curve or displace the peak to the front, that will mimic the behaviour at different stages of the fuel cycle. Normally at the Beginning of Life (BOL), the peak is in the middle of the fuel element, and at the End of Life (EOL) it moves to the front (Fig. 6-1).

Fig. 6-1 Example of normalized heat flux with various $N1$ and $N2$ value

Non-uniform heat fluxes also occur due to large changes of coolant density during the transition from sub- to supercritical conditions. The decrease in density will reduce moderation, the power will decrease in the upper part of the fuel channels, while the

power peak will shift to the lower part of the fuel assembly as described by Tashakor et al. [193].

Table 6-1 List of cases and change of variables in Eq. (40)

Case No.	Variables
Case 1	N/A – uniform heat flux
Case 2	N1=1, N2=1
Case 3	N1=3, N2=1
Case 4	N1=3, N2=0.6
Case 5	N1=3, N2=0.2

Five cases were investigated with the only variable parameters being $N1$ and $N2$. Table 6-1 shows a list of the cases and variable values. The reference case (case 1) is characterized by a uniform heat flux.

6.2.2 Governing Equations

Governing equations are the representation of the fluid flow, the most important being conservative equations of mass, momentum and energy as described in ANSYS Theory Guide [194]. The *Low-Reynolds Shear Stress Transport (SST) $k - \omega$* [88] was used to perform the turbulent model calculations. Palko and Anglart [158] and Wen and Gu [195] also found this model predicted HTC accurately in the supercritical flow, and independently calculated bulk flow ($k - \varepsilon$) and the region close to the wall ($k - \omega$). More information can be found in Chapter 3.

6.2.3 Fluid Properties

The properties of CO₂ at various conditions are taken from The National Institute of Standards and Technology (NIST). “NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)” [81] compiles data for many different fluids at sub- and supercritical conditions including carbon dioxide and water. The used REFPROP is version 9.1. At the transition point from sub- to supercritical conditions, the

fluid parameters change significantly. For example, the rapid change of CO₂ properties at 8.35 MPa is shown in Fig.6-2.

Fig. 6-2 Properties of CO₂ at 8.35MPa

6.2.4 Geometry and Operational and Boundary Conditions

When supercritical CO₂ flows through a vertical pipe, a non-uniform flux is applied at the wall. Since the flow is vertical, the problem can be simplified to 2D axisymmetric geometry, which significantly reduces computational time. The scheme of the geometry and boundary conditions is presented in Fig. 6-3. The hexagonal mesh consists of the following boundary conditions: mass flow inlet, pressure outlet, axis and wall (where the heat flux is applied).

Fig. 6-3 Scheme of the experiment

The computational domain consists of three fluid zones, i.e. two non-heated walls at the inlet and at the outlet, and one heated wall in between. The additional zones were created to make sure that the results at the heated zone will not be influenced by the development of the flow. Hence, the dimensions of the pipe are: a radius of 4 mm with a total length of 2.12 m, where only 1.94 m is the heated wall.

Table 6-2 Scaling parameters [169]

Parameter	Relationship
Pressure (p)	$\left(\frac{p}{p_{cr}}\right)_{water} = \left(\frac{p}{p_{cr}}\right)_{CO_2}$
Temperature (T)	$\left(\frac{T}{T_{cr}}\right)_{water} = \left(\frac{T}{T_{cr}}\right)_{CO_2}$
Heat flux (q'')	$\left(\frac{qD}{k_b}\right)_{water} = \left(\frac{qD}{k_b}\right)_{CO_2}$
Mass flux (G)	$\left(\frac{GD}{\mu_b}\right)_{water} = \left(\frac{GD}{\mu_b}\right)_{CO_2}$

The simulations were conducted with the different heat flux curves, where the average value is identical in every case, as for the mass flux calculations. The investigation aimed to predict if a non-uniform heat flux may lead to pipe overheating at the heat flux peak.

Using fluid-to-fluid scaling parameters for the inlet conditions, the operational and boundary conditions can be set. Table 6-2 shows the major scaling parameter based on pseudo-critical point values.

Table 6-3 Scaling values between fluids

Parameter	Relationship
Pressure (P)	$\frac{P_{water}}{P_{CO_2}} = 1.056$
Temperature (T)	$\frac{T_{water}}{T_{CO_2}} = 2.13$
Heat flux (q'')	$\frac{q_{water}}{q_{CO_2}} = 4.5$
Mass flux (G)	$\frac{G_{water}}{G_{CO_2}} = 0.75$

The aforementioned relations could be used to obtain the boundary conditions for simulation with supercritical CO₂ based on an experiment conducted by Shitsman (1963) [196] for supercritical water. Hence scaling had been performed to create the conditions for the current simulations. Table 6-3 shows the results of the comparison of CO₂ and water critical parameters.

Therefore, the boundary conditions were as follows: an operational pressure of 7.8 MPa; the inlet temperature of 27°C; mass flux of 576 kg/m² s; and heat flux of 71113 W/m². The closest experimental results to the boundary conditions (with the use of CO₂) were found in Zahlan [197], where the operating pressure is 8.35 MPa, the inlet temperature 11°C, mass flux is 700 kg/m² s and heat flux 80 kW/m². Therefore, these parameters were used in further calculations. The experiment of Zahlan [197] and his colleagues used the Super-Critical University of Ottawa Loop (SCUOL).

6.2.5 Convergence Criteria

The convergence criteria for the simulation was set to 10^{-6} for energy and continuity equation, while velocities in the x and y directions, turbulent kinetic energy, and specific dissipation rate have a default value of 10^{-3} . Moreover, cross-sections at different distances from the inlet were monitored, and once constant, the solution has fully converged.

Following ASME CFD recommendations, all equations except turbulent kinetic energy and specific dissipation rate were solved with the use of second order differential schemes, while the last two parameters use the first order scheme. Pressure-velocity was coupled with the SIMPLE scheme.

Published experimental data only provides information about thermal response against uniform heat flux, which does not occur in the real situation. Therefore, an investigation of different non-uniform heat fluxes was conducted to show thermal response at different stages of the fuel cycle.

Fig. 6-4 Comparison of different turbulent models and validation. Case 1, uniform heat flux. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s¹ and heat flux is 80 kW/m²

Mesh validation is shown in Fig. 6-4. The default mesh was created with 125 intervals along the radius and 1mm cell size in the axial direction. It was found that $k-\omega$ SST turbulent model is the most accurate among two-equation models. Further optimization of the mesh allowed a decrease in the number of intervals in the radial direction without sacrificing accuracy. The mesh validation was performed with the use of three meshes with a different number of nodes in the radial direction. In the axial direction, the number of nodes is constant in all meshes, since the sensitivity was found to be negligible in this direction. The final mesh consists of 100 nodes in the radial direction with progressive refinement, where the first cell distance from the wall is equal to 0.002 mm, to make sure that the y^+ value is lower than unity.

6.2.6 Heat Transfer Coefficient

Researchers have for many years been trying to create a relation to predict the heat transfer coefficient (HTC) accurately. In the case of supercritical fluid flow, numerous formulae were derived.

Dittus-Boelter in 1930 [180] proposed a relation for a Nusselt number that is the most commonly used in subcritical flows:

$$\mathbf{Nu} = 0.023\mathbf{Re}^{0.8}\mathbf{Pr}^n \quad (41)$$

It is valid for a pipe length to diameter ratio of $L/D_H > 60$, Reynolds number $\mathbf{Re} > 10000$ and Prandtl number $0.7 < \mathbf{Pr} < 100$. However, it was found that this correlation lacks accuracy at supercritical conditions, and superior models were needed. Two derivations of the Nusselt number can be distinguished, i.e. modification of the Dittus-Boelter equation (the most common) or a more empirical approach.

The rapid change of properties during the transition from sub- to supercritical conditions led Swenson et al. in 1965 [172] to propose a different approach in the definition of the HTC, which resulted in the following equation:

$$\mathbf{Nu} = 0.00459 \left(\frac{DG}{\mu_w} \right)^{0.923} \left(\frac{H_w - H_b \mu_w}{T_w - T_b k_w} \right)^{0.613} \left(\frac{\rho_w}{\rho_b} \right)^{0.231} \quad (42)$$

where D is the diameter, G the mass flux, μ the viscosity, H the enthalpy, T the temperature, k the thermal conductivity, and ρ the density. The sub-indexes w and b stand for wall and bulk parameters, respectively.

Mokry et al. in 2011 [198] modified the Dittus-Boelter formula, hence the Nusselt number was defined as follows:

$$\text{Nu} = 0.0061 \text{Re}^{0.9} \overline{\text{Pr}}^{0.68} \left(\frac{\rho_w}{\rho_b} \right)^{0.56} \quad (43)$$

However, this correlation was developed for supercritical water.

Bishop et al. [199] in 1964 proposed a correlation that takes into account the position along the tube:

$$\text{Nu}_x = 0.0069 \text{Re}_x^{0.9} \text{Pr}_x^{0.66} \left(\frac{\rho_w}{\rho_b} \right)_x^{0.43} \left(1 + 2.4 \frac{D}{x} \right) \quad (44)$$

where D is the diameter of the pipe and subscript x is an axial position.

The most recent formulae were developed by Gupta et al. in 2011 and 2013 [200]. Both correlations were developed based on empirical experiments with the use of H₂O and CO₂. The correlation for H₂O (Gupta 2011) is as follows:

$$\text{Nu} = 0.0033 \text{Re}^{0.94} \overline{\text{Pr}}^{0.76} \left(\frac{\rho_w}{\rho_b} \right)^{0.16} \left(\frac{\mu_w}{\mu_b} \right)^{0.4} \quad (45)$$

while the equation developed for CO₂ is:

$$\text{Nu} = 0.0038 \text{Re}^{0.96} \overline{\text{Pr}}^{-0.14} \left(\frac{\rho_w}{\rho_b} \right)^{0.84} \left(\frac{\mu_w}{\mu_b} \right)^{-0.22} \left(\frac{k_w}{k_b} \right)^{-0.75} \quad (46)$$

Both equations were compared for accuracy in given cases.

6.3 Results

The results show the temperature distribution in all five investigated cases, together with a comparison of the different approaches in calculating the heat transfer coefficients (HTC). These are followed by property analyses along the radius at various distances from the inlet.

6.3.1 Temperature Distribution

The results of the wall temperature distribution in all cases are collected in Fig. 6-5. In the reference case 1, the wall temperature increases steadily along the axis, as there is no HTD effect, whereas the other cases can be characterized by higher temperatures. Especially, in cases 2, 3 and 4, it is very easy to notice that the HTD is presented and its occurrence moves towards the front part of the pipe as the $N1$ parameter increases, hence the temperature peak is closer to the inlet.

Fig. 6-5 Wall temperature in cases from 1 – 5. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s⁻¹ and heat flux is 80 kW/m²

The highest normalized peak of the heat flux is in case 3. By changing the $N2$ value, the peak temperature decreases as shown. On the other hand, case 2 is very interesting, as the heat flux is sinusoid, but the peak wall temperature moves from the middle to the back of

the pipe. In cases 2 to 5, the wall temperature decreases significantly at the end of the pipe and is lower than in case 1.

6.3.2 Heat Transfer Coefficient Distribution

The HTC distribution in the reference case 1 (Fig. 6-6) was validated against experimental results and compared with several published formulae. It can be observed that close to the front part of the pipe, all of the approaches to find HTC fail to predict the trend, while the experimental results show rather constant behaviour. It was not possible to determine which approach is better in the estimation of HTC, but Swenson's et al. formula has the best agreement with the results. However, the numerical approach is superior for following the flow behaviour (except at the inlet).

Fig. 6-6 Analytical, numerical and experimental results comparison of HTC in reference case 1, uniform heat flux. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s¹ and heat flux is 80 kW/m²

Figure 6-7 shows where the heat transfer coefficient has the smallest value and infers where HTD can be observed in particular cases. The decrease of HTC close to the pipe inlet is neglected in developing this conclusion, since the validation against experimental results shows that in this region, the numerical results do not follow the trend. It is

straightforward to predict that the HTC will have the lowest peaking value in case 3, whereas in reference case 1, the HTC is nearly uniform. Cases 2, 3 and 4 shows where HTD occurs. The HTC is characterized by a lower number of positions where the wall temperature increases. The peak value moves towards the front of the pipe as the $N1$ parameter increases. HTC of non-uniform heat flux cases is characterized by lower values at the part where the normalized heat flux is higher than unity. The HTD is always followed by a rapid increase of HTC (as the heat flux decreases) and its value at the outlet is significantly higher than the reference case.

Fig. 6-7 HTC in cases from 1 – 5. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s⁻¹ and heat flux is 80 kW/m²

Comparison of the analytical and numerical approaches in calculating the HTC of case 3 is presented in Fig. 6-8. All HTC correlations can predict HTD placements with a decrease of HTC at about 0.5 m. At the inlet (which was neglected before), all solutions, except Dittus-Boelter, show similar behaviour, i.e. the HTC decreases. While the agreement is rather consistent before and during HTD, towards the end, the results are increasingly divergent. The Guptas's et al. (2013) formula derived for supercritical CO₂ consistently under predicts, whereas all other correlations tend to over predict, making it

difficult to conclude which formula is most appropriate. However, before HTD, Swenson's et al. formula is superior.

Fig. 6-8 Analytical and numerical results comparison of HTC in case 3, $N = 3$, $N_2 = 1$. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s⁻¹ and heat flux is 80 kW/m²

6.3.3 Property Analysis

The focus in this section is on the most interesting case, i.e. case 3, which is characterized by the highest peak wall temperature. The radial distribution of velocity is shown in Fig. 6-9, and shows the narrowest peak of fluid velocity near the position where HTD is observed (500 mm). The bulk velocity becomes progressively uniform with the axial distance, although the flow close to the wall always has a higher velocity.

The viscosity distribution along the radius (Fig. 6-10) shows a decrease of the value closer to the wall, with a rapid small peak adjacent to the wall. However, the peak occurs only close to the inlet but at greater distances, it disappears. The highest peak is at a distance of 400 mm from the inlet, however, at 300 mm from the inlet, the slope of the change is the highest and almost linear. With greater distances from the inlet, the viscosity fluctuations diminish, and at 700 mm from the inlet, the viscosity differs nearly only next to the wall.

Fig. 6-9 Velocity distribution along radius position (mm) in case 3, $N = 3$, $N_2 = 1$. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s⁻¹ and heat flux is 80 kW/m²

Fig. 6-10 Viscosity distribution along radius position in case 3, $N_1 = 3$, $N_2 = 1$. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s⁻¹ and heat flux is 80 kW/m²

The density distribution curves along the pipe radius (Fig. 6-11) have a shape very similar to the distribution of viscosity, but the density differences close to the inlet and after HTD occurs are much smaller than observed for viscosity. Generally, the density

distribution is more uniform than other properties, as seen in other figures. Only close to the wall does the density change significantly.

The specific heat distribution (Fig. 6-12) shows a transition layer from sub- to supercritical fluid exactly and its development along the axis. It appears where the HTD phenomenon occurs and shows the influence of specific heat of the fluid near the heated wall, i.e. the peak of specific heat is wider right before the HTD position. The values of specific heat near the wall are much greater than in the bulk flow, hence they affect the thermal response at this location. Behind the HTD position, the bulk specific heat is significantly higher than at the locations before it.

Fig. 6-11 Density distribution along radius position in case 3, $N1=3$, $N2=1$. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s⁻¹ and heat flux is 80 kW/m²

Fig. 6-12 Specific heat distribution along radius in case 3, $N_1=3$, $N_2=1$. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s¹ and heat flux is 80 kW/m²

Fig. 6-13 Thermal conductivity along radius position in case 3, $N_1=3$, $N_2=1$. Operating pressure is 8.35 MPa, the inlet temperature is 11°C, mass flux is 700 kg/m² s¹ and heat flux is 80 kW/m²

The thermal conductivity (Fig. 6-13) behaves similarly to the velocity and specific heat, and show a characteristic peak value near the wall. However, after this peak, the value rapidly decreases and then slowly increases. At a greater distance (700 mm), the bulk thermal conductivity has the lowest value as the conductivity decreases with the temperature, whereas the peaking value has a similar value at every distance. At the region before the occurrence of HTD, the bulk thermal conductivity is higher than after it.

6.4 Discussion and Conclusions

Numerical investigation of vertical flow in an upward direction was simulated with the use of CFD software, leading to a better understanding of the phenomena occurring during the transition from sub- to supercritical conditions. It was found that the flow is sensitive to any variation in the heat flux distribution along the axis.

It is believed that heat transfer deterioration occurs when the heated wall has much higher temperature than the pseudo-critical temperature of the flowing medium, while the bulk temperature is lower than the pseudo-critical case. This agrees with the present calculations, and show that HTD occurs when a non-uniform heat flux is applied. Therefore, the HTD occurs before peaking values of heat flux due to the temperature difference between the coolant and heated wall being highest.

The wall temperature decreases towards the outlet because the heat flux decreases. Nevertheless, further investigations could be carried out to study this phenomenon since for reactors using supercritical fluid as a coolant, the transition from sub- to supercritical parameters may influence the power distribution along the fuel rod. The high density of coolant at the inlet stage provides good moderation, whereas the supercritical fluid has weaker moderation ability. Hence, the power at the beginning of the channel will be highest.

Comparison of experimental results, numerical calculations, and analytical estimation show that the Swenson's et al. formula is the most reliable in predicting the heat transfer coefficient in case of uniform heat flux. In the non-uniform heat flux case, the heat transfer coefficient is predicted rather accurately by most of the formulae, i.e. the HTC

has been predicted accurately until the point where the heat transfer deterioration occurs, and until this place, Swenson's et al. formula matches the numerical results. After the occurrence of HTD, the HTC increases, however, the analytical solution increases much faster than the numerical solution.

The property analysis shows that, along the radial direction, the specific heat and thermal conductivity are characterized by a rather narrow peak in properties close to the pipe wall. However, towards the centre of the pipe, the flow becomes uniform. Specifically, the peak of the specific heat values is the highest. The HTC is most strongly influenced by the thermal conductivity of the fluid. This property varies differently before and after the occurrence of HTD, i.e. close to the inlet the value of bulk thermal conductivity is higher than the value of bulk flow after the peak value. Therefore, it has the main impact on this phenomenon since the thermal conductivity decreases with the distance from the inlet.

Chapter 7

Numerical Investigation of Supercritical Water Flow in a Vertical Pipe under Axially Non-Uniform Heat Flux*

A numerical investigation of water flow in a vertical pipe during the transition from sub- to supercritical conditions when non-uniform power is applied axially at the wall is presented. The Computational Fluid Dynamics calculations were compared to published experimental results where a uniform heat flux was applied. A high dependency of the wall temperature distribution on the power distribution curve shape was found when the peak heat flux is close to or behind the heat transfer deterioration (HTD) phenomenon. However, if the peak moves to the front of the pipe, lower temperatures are achieved compared to the uniform heat flux. Nusselt number calculations for convective heat transfer found Bishop's and Ornatsky's formulae followed the experimental observations. Sensitivity calculations demonstrated that the wall temperature is much more dependent on the mass flux, than the operating pressure, with higher temperature variation accompanied by positional displacement of the HTD.

*This section published substantially as reference: Rowinski et al. "Numerical investigation of supercritical water flow in a vertical pipe under axially non-uniform heat flux." Progress in Nuclear Energy 97: 11-25.

7.1 Introduction

Super-Critical Water-cooled Reactors (SCWRs) are one of the most promising technologies accepted by Generation IV International Forum (GIF) [119, 201], that are under development worldwide, due to the possibility of increasing light water reactors' (LWRs) efficiency from the current ca. 35% to ca. 48%. Specifically, the steam is delivered under much higher temperature and pressure than in contemporary reactors, i.e. above the pseudo-critical point, and similar to the current fossil fuel thermal power plants. Oka and other researchers are designing reactors to make this technology operational [103, 132, 202, 203] for both large (1000 MW_{el} [204]) and small (300 MW_{el} [205]) reactors. From a thermal-hydraulics viewpoint, one challenge is to fully understand the transition from sub- to supercritical conditions. Duffey and Pioro [171] reviewed most significant experiments with supercritical water flow inside pipes, annuli, and fuel rod bundles, and reported only two experiments of the rod bundle type including the work of Wang et al. [206]. Although, the amount of experimental data is limited, Computational Fluid Dynamics (CFD) codes can simulate supercritical flow successfully. In recent years, numerical methods have been validated against literature data, e.g. by Jaromin and Anglart [207] or Gu et al. [208].

Nevertheless, these experiments or simulations were performed only when uniform heat flux was applied at the wall. In the real situation, the heat flux in the fuel rod is non-uniform and should be included during evaluation. Only Wang et al. conducted an investigation where a circumferentially non-uniform heat flux was applied at the pipe wall [209], however, in a Reactor Pressure Vessel (RPV), the power generated in the fuel assembly is non-uniform axially. Water properties on either side of the pseudo-critical point are significantly different. From the power generation point of view, the density is the most influential. During the transition from sub- to supercritical conditions, the fluid density decreases significantly (almost one order of magnitude) and therefore, at the inlet of the fuel assembly, moderation is much greater than at the outlet. Tashakor et al. [193, 210] performed an evaluation of power distribution along the fuel rods and found that the power distribution in the axial direction has a sinusoidal shape with its peak moved the upstream section of the fuel assembly to around 15% of the total fuel rod length.

Fig. 7-1 Thermal properties of water at 25.5 MPa

The main thermal properties of the water at 25.5 MPa are shown in Fig. 7-1. When pressure is above the critical point, boiling does not occur with an increase of the temperature, and the properties change continuously. This is especially for the specific heat whose peak near the pseudo-critical point is around 15 times higher than elsewhere. The other parameters are ca. 5-8 times lower at supercritical conditions than at subcritical temperature. Thermal conductivity can be characterized with a small peak just before the pseudo-critical point, whereas viscosity is the lowest right after the pseudo-critical point then slightly increases with temperature. Nevertheless, viscosity is much lower than at subcritical conditions. The only parameter that continuously decreases with temperature is density.

Despite the absence of a boiling crisis, the heat transfer deterioration (HTD) phenomenon in specific conditions may lead to an undefined rise in peak cladding temperature (PCT). HTD remains incompletely defined at present, and therefore, the current research focuses on the HTD mechanism and avoiding HTD. Sometimes the enhancement of heat transfer

(EHT) occurs, however, to be conservative in the safety analysis, this is not being taken into account. Historically, NPP safety estimates were conservative and were evaluated with wide safety margins to accommodate the worst possible scenarios. Nowadays, the nuclear industry and research tend to use best estimate methods such as CFD computations with uncertainty evaluation.

The study was conducted using the ANSYS Fluent code. The geometry consisted of a fluid volume with the following boundary conditions: mass flow inlet, pressure outlet, axis and wall. The mesh was validated against available data with uniform heat flux. The non-uniform heat flux was programmed in a User Defined Function (UDF) file based on the position in the axial direction. The turbulence model used in the numerical investigation was low-Reynolds $k-\omega$ Shear Stress Transport (SST), due to its proven ability to accurately simulate supercritical flow [158, 195]. Numerical investigations answer how the wall temperature distribution along fuel rod behaves under non-uniform heat flux at the wall. The MCST cannot exceed safety limits during operation and therefore, it has to be proven that under non-uniform heat flux it is possible to achieve the required outlet temperature without sacrificing any of the safety criteria.

7.2 Methodology – Numerical Approach

Since the experimental investigation is expensive and requires building a facility able to perform either scaled or non-scaled experiments, it is convenient to use numerical methods. The numerical methods also avoid the need for expensive instrumentation to collect data during the tests. The use of computer analysis is cheaper and more efficient as computational power is readily increasing. Therefore, the use of a numerical approach at the early design stage is appropriate.

Computational Fluid Dynamics (CFD) is commonly used and is a powerful tool to predict with satisfactory accuracy experimental phenomena. Hence, many researchers perform calculations using commercial or self-developed CFD software. More information about CFD was provided in Chapter 3.

The water properties during the transition from sub- to supercritical conditions vary significantly and therefore, may affect the accuracy of calculations. The “NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)” [81]

contains property data tables of many different fluids at sub- and supercritical conditions including water and carbon dioxide relevant to Generation IV nuclear reactors. The water properties are based on the work conducted by Kestin et al. [211, 212] and Sengers et al. [213, 214], and are based on Helmholtz free energy. Thus, it is possible to either create an UDF with water properties or use the NIST real gas model. Since ANSYS Fluent has incorporated the REFPROP version 9.1 database, this software was used to perform the calculations.

The solver used to perform pressure based calculations uses the SIMPLE scheme, where second order discretization for pressure, density, momentum, and energy solved the main governing equation, while a first order scheme was used for turbulent kinetic energy and specific dissipation rate. To ensure sufficient accuracy convergence, criteria were set to residuals of 10^{-6} for continuity and energy.

7.2.1 Axial Power Distribution

Heat flux distribution is a reflection of power generation inside the fuel element, and depends on burn-up, enrichment variation, moderation, and a burnable neutron absorber. Because fission in nuclear fuel occurs more rapidly when sufficient moderation is provided, in typical PWRs, the power curve is sinusoid with a peak in the middle of the fuel channel. However, in SCWRs during the transition from sub- to supercritical conditions, the density decreases significantly and therefore the moderation decreases towards the outlet. This phenomenon causes the peak of power distribution to move from the middle position towards the channel inlet (as shown by Tashakor et al. [210]). See Fig. 7-2.

Fig. 7-2 Normalized axial power along the fuel assembly height [210]

In PWRs during different stages of the fuel cycle, the power distribution is changing and the peak moves towards the inlet, similar to the predicted distribution for SCWR. As described in Chapter 6, Blakeman's and March-Leuba's [192] formula was used for 5 different cases as presented in Table 7-1.

Table 7-1 Values of $N1$ and $N2$ for different investigated case

Case No.	Variables
Case 1	N/A – uniform heat flux
Case 2	$N1=1, N2=1$
Case 3	$N1=4, N2=1$
Case 4	$N1=4, N2=0.6$
Case 5	$N1=4, N2=0.2$

The normalized heat flux distribution is shown in Fig. 7-3

Fig. 7-3 Normalized heat flux distribution along the axis with different $N1$ and $N2$ values

Fig. 7-4 Geometry and boundary conditions of fuel walls (dimensions in mm, model is unscaled)

7.2.2 Geometry

The computational domain was simplified from the full 3D model to a 2D axisymmetrical geometry in order to optimize computational time. It is possible due to the shape of the model and the direction of the applied forces, i.e. gravity and mass flux, and is based on the Ornatsky experiment [215], i.e. the vertical pipe of 1.05 m in length and 3mm in diameter (Fig. 7-4), as it is within the operating parameters of a typical SCWR. To ensure that the results would not be influenced by flow development, two additional domains of length of 50 mm at the inlet and the outlet were added. Therefore,

the flow is developed at the inlet to the heated region and bulk flow at the outlet can stabilize.

The geometry was created and meshed with GAMBIT software, and validated both in the radial and axial directions. In every mesh, the main criterion was to obtain a y^+ value below unity to ensure the numerical investigation is accurate. This is necessary because the *Low-Reynolds $k - \omega$ SST* turbulent model does not use any wall functions. Since y^+ can be defined as the non-dimensional distance between the wall and the first computational node, the first node was placed 0.0005 mm from the wall. Therefore, the y^+ value varies in the range from 0.3 – 0.7.

First, the validation was performed in the radial direction (Fig. 7-5). A mesh of 125 interval counts in the radial direction was chosen, since the result was placed between meshes of 150 and 175 interval counts, and it is sufficiently precise to compare with the experimental data. The difference between 125 and 150 meshes was negligible. In the axial dimension, three meshes were investigated, with interval sizes of 0.5 mm, 1 mm and 2 mm (Fig. 7-6), with the latter having the best accuracy. Therefore, for all computations, a mesh with 125 interval counts in the radial direction and interval size of 2 mm in the axial direction was used.

Fig. 7-5 Mesh comparison in the radial direction. Different interval count. Case 1, uniform heat flux. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Fig. 7-6 Mesh comparison in the axial direction. Different interval size. Case 1, uniform heat flux. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

7.2.3 Boundary and Operating conditions

Boundary and operating conditions were taken from the Ornatsky experiment, and a simplified diagram is shown in Fig. 7-4. The following boundary conditions were set: mass flow inlet, pressure outlet, axis and wall (where heat flux is applied). In all cases, the mass flux (G) of $1500 \text{ kg/m}^2 \text{ s}$, inlet temperature (T_{in}) of 96°C and gravity acceleration of 9.81 m s^{-2} is constant, and only the heat flux (q'') varies. The reference case 1 is characterized by uniform q'' of 1810 kW/m^2 , while the remaining cases are non-uniform as was explained in section 2.1. The heat flux was normalized to achieve an average q'' as in the reference case. The operating pressure is 25.5 MPa and above the critical point.

The Heat Transfer Coefficient (HTC) was calculated according to the following equation:

$$h = \frac{q''}{T_w - T_b} \quad (47)$$

where q'' is the heat flux, T_w the wall temperature, and T_b the local bulk temperature.

The Nusselt number is calculated as follow:

$$\text{Nu} = \frac{hL}{k} \quad (48)$$

where h is the HTC calculated from Equation 43, L the characteristic length (hydraulic diameter in our calculations), and k the bulk thermal conductivity.

7.2.4 Convective Heat Transfer

Many empirical and semi-empirical correlations have been formulated to predict the heat transfer coefficient in the supercritical flow. Therefore, the numerical investigation is followed by a comparison of experimental and simulation results with six correlations to identify those best predicting the obtained values of Nusselt number, and hence the HTC.

The most common relation for the Nusselt number was proposed by Dittus-Boelter [180]:

$$\text{Nu} = 0.023 \text{Re}^{0.8} \text{Pr}^n \quad (49)$$

It is valid for ratio of pipe length to diameter $L/D_H > 60$, Reynolds number $\mathbf{Re} > 10000$ and Prandtl number $0.7 < \mathbf{Pr} < 100$. The exponent n is equal to 0.4 for heating and 0.3 for cooling. The properties should be estimated at mean temperature, i.e. bulk temperature. In the present calculations, the n exponent has a value of 0.4. Although this correlation was not developed specifically for supercritical flow estimation, it is used here for comparison since it is the most commonly used formula for the computation of HTC in the case of forced convection in turbulent flows.

For many years, a formula has been sought that is valid for both sub- and supercritical regions, leading to two modifications of Dittus-Boelter's equation and new correlations.

In 1957, Shitsman [172] proposed a new formula based on the Dittus-Boelter relation:

$$\mathbf{Nu} = 0.0243 \mathbf{Re}_b^{0.8} \mathbf{Pr}_{\min}^{0.8} \quad (50)$$

where $\mathbf{Re}_b$ stands for Reynolds number calculated at bulk fluid temperature and $\mathbf{Pr}_{\min}$ denotes the Prandtl number calculated at either bulk fluid temperature or the wall surface temperature, depending on which is smaller.

Krasnoshchekov and Protopopov in 1959 [172] proposed a new formula for forced convective heat transfer in water and carbon dioxide (CO_2):

$$\mathbf{Nu} = \mathbf{Nu}_0 \left(\frac{\mu_b}{\mu_w} \right)^{0.11} \left(\frac{k_b}{k_w} \right)^{-0.33} \left(\frac{\bar{c}_b}{c_{pw}} \right)^{0.35} \quad (51)$$

where

$$\mathbf{Nu}_0 = \frac{(\xi/8) \mathbf{Re}_b \bar{\mathbf{Pr}}}{12.7 \sqrt{(\xi/8)} (\bar{\mathbf{Pr}}^{2/3} - 1) 1.07} \quad (52)$$

and

$$\xi = \frac{1}{(1.82 \log_{10} \mathbf{Re}_b - 1.64)^2} \quad (53)$$

where subscript b stands for evaluation at bulk temperature, and w stands for evaluation at wall temperature. The Prandtl number and specific heat should be averaged over the ranges of thermophysical variations. The above correlation is valid for pressure of 22.3 – 32 MPa for water and 8.3 MPa for CO₂.

Another common correlation for the Nusselt number is the one developed by Bishop et al. [199] proposed in 1964. The correlation was based on experiments done under following conditions: pressure in the range of 22.8 – 27.6 MPa, bulk temperature of 282 – 527 °C, mass flux of 651 – 3662 kg m⁻² and heat flux of 0.31 – 3.46 MW m⁻². It is given by:

$$\text{Nu}_x = 0.0069 \text{Re}_x^{0.9} \text{Pr}_x^{0.66} \left(\frac{\rho_w}{\rho_b} \right)_x^{0.43} \left(1 + 2.4 \frac{D}{x} \right) \quad (54)$$

where D is the diameter of the pipe and x is an axial position.

Swenson et al. in 1965 [172] had found that standard correlation for HTC is not valid in a rapid change of properties during the transition from sub- to supercritical environment and therefore the following expression is recommended:

$$\frac{hD}{k_w} = 0.00459 \left(\frac{DG}{\mu_w} \right)^{0.923} \left(\frac{(H_w - H_b)\mu_w}{(T_w - T_b)k_w} \right)^{0.613} \left(\frac{\rho_w}{\rho_b} \right)^{0.231} \quad (55)$$

The following ranges of experimental results were used to develop the correlation: pressure of 22.8 – 41.4 MPa, mass flux of 542 – 2150 kg m⁻²s⁻¹, wall temperature of 93 – 649 °C and bulk fluid temperature of 75 – 576 °C. Hence, it covers the greatest spectrum of the results, and yields good accuracy with CO₂.

Ornatsky et al. in 1970 [215] proposed a variation of Shitsman's relation as follow:

$$\text{Nu} = 0.0243 \text{Re}_b^{0.8} \text{Pr}_{\min}^{0.8} \left(\frac{\rho_w}{\rho_b} \right)^{0.3} \quad (56)$$

where subscript b stands for evaluation at bulk temperature and w for evaluation at wall temperature based on experimental data.

7.3 Results and discussion

The results provide information on how the wall temperature responds to uniform and non-uniform heat flux. The main emphasis is on the correlation between the wall temperature and heat transfer coefficient in particular cases. The numerical results are compared with the prediction of convective heat transfer coefficient calculated as described in section 6.2.4.

Fig. 7-7 HTC and temperature distributions against distance from the inlet. Reference case 1 Case 1, uniform heat flux. Operating pressure is 25.5 MPa, the inlet temperature is 96 C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

7.3.1 Uniform Heat Flux

Temperature and HTC

The uniform heat flux computation is a benchmark case for the results with non-uniform heat flux. Case 1 shows (Fig. 7-7) the distribution of heat transfer coefficient (HTC) and temperatures distribution along the pipe in the reference case, where the heat flux is constant. The rapid changes of HTC and wall temperature at the inlet and the outlet arise because the heated wall is connected to two unheated faces and therefore are not considered further. The wall temperature distribution at the entrance of the pipe increases linearly and, at around 0.6m from the inlet, the temperature rises quickly as HTC

decreases, i.e. the HTD phenomenon occurs. However, once the HTC stabilizes then begins to increase again, the temperature starts to decrease before the outlet. The peak wall temperature is 529.7°C , while the bulk temperature increases nearly linearly with the distance from the inlet.

Fig. 7-8 Comparison of numerical investigation results with analytical prediction and with Ornatsky results. Case 1, uniform heat flux. Operating pressure is 25.5 MPa, the inlet temperature is 96°C , mass flux is $1500 \text{ kg/m}^2 \text{ s}$ and heat flux is 1810 kW/m^2

HTC Investigation

The comparison results of the Nusselt number between the Ornatsky et al. experimental results, numerical and analytical investigation are shown in Fig. 7-8. Numerical results tend to slightly under estimate the convection effect, but are closest to Ornatsky's et al. experiments (uniform heat flux) over the whole range of coolant enthalpy. While most of the analytical solutions are able to predict the place where HTD occurs (except Dittus-Boelter's and Shitsman's et al. correlations), the results are usually over estimated. Swenson's et al. correlation is the best example of over estimation, while most of the correlations can be characterized by small peak immediately before HTD, this shows a 3 – 4.5 times higher peak. The Krasnoshchekov and Protopopov's formula over predicts

the results while the trend of HTD is preserved. The Bishop's et al. and Ornatsky's et al. formulae are the most accurate in the case of analytical analysis. In the subcritical region both show very good agreement with experimental data, while after HTD they tend to over predict the convective heat transfer. However, the Bishop's et al. correlation shows the result to be closer to the experiment in a higher range of coolant enthalpy.

7.3.2 Non-uniform Heat Flux

The results of non-uniform heat flux, i.e. cases 2 – 5, as presented in this section, demonstrate that it is possible to achieve lower maximum wall temperatures. Nevertheless, the outlet temperature in every case is the same, i.e. 387°C. As it was shown in Fig. 7-3, the heat flux at the inlet and outlet are zero, hence the values do not change rapidly at those points when non-uniform heat flux is applied. This investigation emphasizes on the wall temperature distribution, but the conduction heat transfer from the heated region to the unheated regions is excluded.

Fig. 7-9 HTC and temperature distributions against distance from the inlet. Case 2, $N1=1$, $N2=1$. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Temperature and HTC

Case 2 (Fig. 7-9) shows the highest maximum wall temperature among all considered cases, i.e. 844.41°C, as expected since the peak heat flux value in the middle of the pipe

is near where HTD is most likely to occur. HTD is evident around 0.5 m from the inlet, hence with rapid decrease of HTC, as the wall temperature increases rapidly with a peak at around 0.7m from the inlet. Then the temperature decreases with the swift increase of HTC towards the outlet.

The heat flux in case 3 (Fig. 7-10) has higher peak value than in case 2, however, due to the fact that it is moved to the front, the maximum wall temperature is more than 100°C lower (727.68°C). Nevertheless, it is still significantly higher than the reference case. The decrease of the HTD is smoother than in case 2, moreover, the bulk critical temperature is achieved closer to the inlet, and the peak wall temperature is around 0.3 m from the inlet.

Fig. 7-10 HTC and temperature distributions against distance from the inlet. Case 3, $N1=4$, $N2=1$. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Although the peak heat flux in case 4 is not the lowest and it is placed at the inlet region similar to case 3, the HTC is steady and constant until about 0.45 m from the inlet where HTD is observed (Fig. 7-11). The maximum wall temperature can be found at a 0.5 m distance from the inlet, and is slightly higher than in the reference case, where uniform heat flux was applied and the value is 544.85°C.

Fig. 7-11 HTC and temperature distributions against distance from the inlet. Case 4, $N1=4$, $N2=0.6$. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Fig. 7-12 HTC and temperature distributions against distance from the inlet. Case 5, $N1=4$, $N2=0.2$. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Figure 7-12 shows the correlation between temperature and HTC in case 5. This case is characterized by the most uniform heat flux and the lowest maximum wall temperature among the investigated cases with non-uniform heat flux. The maximum value of 503.08°C is lower than all other investigated cases including the reference case, and occurs at around 0.6 m from the inlet followed by a rather rapid decrease of temperature.

HTC Investigation

The results of the Nusselt number calculations were used to compare the analytical solutions proposed by different researchers and the results obtained during the numerical investigation of case 3 (Fig. 7-13). Again, the Dittus-Boelter's correlation is unable to predict the HTD phenomenon. This time, Shitsman's formula is more satisfactory but the Nusselt number is over estimated for the whole enthalpy range. Swenson's et al. correlation shows a high peak near the HTD position which is followed by under prediction of the results after HTD occurs. The Krasnoshchekov and Protopopov's formula overestimates the convective heat transfer in the whole spectrum of enthalpy, however, it approximately predicted HTD. Again, Bishop's et al. and Ornatsky's et al. formulae show the best agreement with the simulation results. However, it is unable to choose the best correlation since the Bishop's formula is more accurate at the lower enthalpy range while Ornatsky's et al. correlation follows the trend in higher ranges.

Properties Distribution

Similar comparisons were done for the bulk flow. Figure 7-14 shows how the bulk flow properties vary downstream. Reference case 1 (top) and case 3 looks very alike, the main difference is the range of particular properties and how fast they change, especially the specific heat maximum value in case 3 is nearly twice the reference case. It can be noticed that in the reference case, the specific heat at the outlet does not reach a peak point, whereas in case 3 it can be observed that the curve has sinusoid-like shape and is about to change direction or stabilize. All other properties reach their minimum values at the outlet. In case 3, the properties tend to stabilize at the exit.

Fig. 7-13 Comparison of numerical investigation results with analytical prediction in case 3, $N1=4$, $N2=1$. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Case 3 is interesting since the heat flux distribution is the closest to the power distribution found in the calculations of Tashakor et al. [210]. Therefore, comparison of the properties distribution along the pipe wall between case 1 (top) and case 3 (bottom) is shown in Figure 7-15. In each case, the peak of specific heat indicates where the transition from sub- to supercritical at the wall occur and moreover it indicates where HTD starts. Other properties, i.e. thermal conductivity, viscosity and density rapidly decrease during the transition. When non-uniform heat flux is applied on the wall, the properties fluctuate downstream after the occurrence of HTD, whereas, the properties downstream are rather constant when uniform heat flux is applied. The differences are especially visible close to the outlet of the investigated domain. In case 3, it is possible to distinguish the second peak of specific heat at the pipe exit, because when the heat flux tends to zero the specific heat approaches the bulk flow value.

Fig. 7-14 Bulk flow properties distribution, case 1 (top) and case 3 (bottom). Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Fig. 7-15 Properties distribution along the pipe wall, case 1 (top) and case 3 (bottom). Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 $\text{kg/m}^2 \text{s}$ and heat flux is 1810 kW/m^2

The comparison of radial fluid property distributions at different axial positions between case 1 and case 3 is shown in Fig. 7-16. The radius distance is normalized and limited only to the part of interest close to the wall, where the properties vary the most. The first cross sections at distances of 600 mm and 150 mm (case 1 and case 3, respectively) from the inlet are located roughly where HTD occurs. The following cross sections are located at the early phase of HTD where the highest temperature occurs and the wall temperature begins to decrease. The values of specific heat are higher in case 1, especially at the last measured cross section. Moreover, the peak's width at each axial location is wider. The peaks at the first two locations in case 1 are very similar, whereas the peak at the second location in case 3 is lower than at the first location. The bulk specific heat increases downstream.

Viscosity behaves very similarly in both described cases. However, the values in case 1 are most similar to each other and have lower values. The case 3 values have a wider spread and are 15-20% higher. Close to the wall, the property values decrease only to increase rapidly near the pipe centre at all locations (except the first one). The most significant difference is the fact that this decrease in values is more significant in case 3. The bulk viscosity decreases downstream.

Density behaves similarly in both investigated cases, the only difference being that case 3 has higher values. The trend is the same in both cases. With bulk density decreasing downstream.

Thermal conductivity follows viscosity, and case 3 is characterised by wider spread and higher values in general, and also shows a small decrease close to the wall. The rapid increase of thermal conductivity is followed by an almost instant stabilization. Again, the bulk values decrease downstream.

Fig. 7-16 Radial distribution of fluid properties at different axial locations in case 1 (left) and case 3 (right). Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 $\text{kg/m}^2 \text{s}$ and heat flux is 1810 kW/m^2

7.3.3 Mass Flux and Pressure Influence

As it was mentioned in the previous subsection, case 3 is the most interesting for this study, and was further investigated to study how mass flux and operating pressure would influence the wall temperature distribution. In both cases, the values vary from -5% to +5% from the reference values.

Fig. 7-17 Wall temperature dependence on mass flow in case 3, $N1=4$, $N2=1$. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

Variation in mass flux from 1425 to 1575 kg m⁻² s⁻¹ influences the temperature distribution significantly (Fig. 7-17). Especially, the lower coolant flow causes a high rise in temperature distribution and moves the HTD phenomenon closer to the pipe inlet. The maximum wall temperature is 884°C.

The operating pressure has less influence on the wall temperature distribution than the variation of the mass flux. As it is shown in Fig. 7-18, the maximum temperature barely achieves 833°C at an operating pressure of 26.775 MPa, while the HTD phenomenon occurs at almost the same position as with the default operating pressure.

Fig. 7-18 Wall temperature dependence on operational pressure in case 3, $N1=4$, $N2=1$. Operating pressure is 25.5 MPa, the inlet temperature is 96°C, mass flux is 1500 kg/m² s and heat flux is 1810 kW/m²

7.4 Conclusions

The numerical investigation of water flow at supercritical conditions in a vertical pipe at non-uniform heat flux at the wall has led to the following conclusions. The wall temperature distribution along the axis is higher in three cases where non-uniform heat flux was applied as compared to reference uniform case, whereas in only one case the maximum wall temperature was smaller. Therefore, it can be concluded that by adjusting the shape of the heat flux distribution curve, lower temperatures are achieved, assuring higher safety margins. This behavior explained by the heat flux peak moving upstream where the coolant is subcritical and more efficient. Moreover, the heat flux peak is lower. Hence, case 5 has the lowest maximum wall temperature among all cases, including the reference case where uniform heat flux was applied.

The Heat Transfer Deterioration (HTD) phenomenon moves upstream even if the heat flux peak is in the middle of the pipe. The Heat Transfer Coefficient (HTC) behaves differently than in constant heat flux case. The HTC tends to be uniform until the point

where the HTD occurs, whereas when the uniform heat flux was applied the HTC was increasing linearly.

Comparisons between the numerical investigations with analytical solutions and experimental data taken from Ornatsky et al. showed that numerical investigations have advantages. While most analytical methods predict the occurrence of HTD, only Bishop's et al. and Shitsman's correlations follow the trend, but in both cases, the results are over estimated at high enthalpy values. A similar comparison was prepared for case 3, but since no experimental data was available, the comparison is only between numerical and analytical solutions. This time, only Dittus-Boelter correlation was unable to predict the occurrence of HTD. Again, the Bishop's and Ornatsky's et al. correlations are the closest to the numerical solution, however, while Ornatsky's et al. formula over estimates values it follows the trend for the whole range of enthalpy.

The property distributions along the wall differ slightly in two of the compared cases, i.e. when uniform heat flux and non-uniform heat fluxes were applied, the power distribution curve predicted was similar to a real reactor. The specific heat is higher in case 1, however, all other properties are higher in case 3. What is interesting is that the viscosity and thermal conductivity decrease close to the wall in case 3, resulting in less efficient heat removal than in case 1, where the aforementioned properties are either stable or increase slowly close to the wall. Therefore, the maximum wall temperature is higher in case 3.

The sensitivity investigation in the case of mass flux and operating pressure found that the temperature distribution is more sensitive to changes in mass flux, i.e. the Reynolds number. The 5% difference in this parameter changes not only the temperature distribution but also the place where HTD occurs, whereas variation in the operating pressure influences only the temperature distribution along the axis.

Chapter 8

Numerical Investigation of Supercritical Water Flow in a 2×2 Rod Bundle*

Generation III/III+ nuclear reactors use subcritical fluids ($T_{cr} = 373.946^{\circ}\text{C}$, $p_{cr} = 22.064 \text{ MPa}$) that limits heat transfer efficiency. SuperCritical Water-cooled Reactors (SCWRs) offer efficiency improvements of nearly 30% above the current NPPs, and such decarbonized electrical energy sources could achieve an efficiency of 45% and capacity factor of ca. 90%. In a subcritical reactor, a uniform heat flux is generated due to relatively constant fuel moderation, however, density changes during the sub- to supercritical transition lead to uneven fuel moderation. This Chapter describes the simulation of a non-uniform heat flux in a SCWR, to analyse the impact on the working medium flow and suggest ways to mitigate the negative impacts of non-uniform heat flux. It is shown that the shape of heat flux curve along the channel strongly influences the wall temperature distribution along the fuel channel. The differences in maximum wall temperatures can be up to 150°C for different curve shapes. Moreover, the maximum wall temperature is always higher than the default case where a uniform heat flux is applied.

*This section published substantially as reference: Rowinski et al. (2016). “Numerical Investigation of Supercritical Water Flow in a 2x2 Rod Bundle under Non-Uniform Heat Flux”, 24th International Conference on Nuclear Engineering (ICONE), Charlotte, North Carolina, USA.

8.1 Introduction

The SCWR concepts have been investigated since the beginning of the “Atomic Age” however, due to material science limitations, were not deployed at that time. Today, the material science is much more advanced and this concept may become operational in the near future. Therefore, researchers are trying to make this technology a reality by assuring its robustness during operation and accidental conditions. The timing is opportune to introduce more efficient technology since 225 reactors, out of a total of 438 reactors, have been in operation for 30 and more years. Therefore, the Generation IV type reactors can replace old and outdated Generation II and III NPPs.

The numerical investigation of 2×2 rod bundle uses simplified geometry. Only one subchannel is simulated, with the rest being taken into account using the symmetry boundary conditions. This geometry was chosen based on the data of Wang et al., 2014 [206] to validate the created mesh and its behaviour during the transition from sub- to supercritical conditions. The heat flux distribution is a reflection of power generation inside the fuel element, and depends on burn-up, enrichment variation, moderation, and a burnable neutron absorber. Therefore, the investigation of non-uniform heat flux is appropriate and valuable.

8.2 Numerical Model

The numerical investigation was conducted with ANSYS Fluent, which is a well validated CFD code using finite volume methods to solve the Navier-Stokes equations. The National Institute of Standards and Technology (NIST) database is incorporated to provide thermodynamic properties of many fluids including water, which was used for the present calculations.

The CFD calculations are often used in early stage design as an economic alternative to a real experiment, which requires expensive equipment and data acquisition instrumentation. Safety issue is also not a problem while using numerical methods. Despite these advantages, the final models will require validation against empirical results obtained in a test facility.

The setup of the Wang et al. [206] experiment is shown in Fig. 8-1. It is a 2×2 fuel rod bundle. The thermocouples were placed at every 100 mm intervals and the measurements

used to validate the present model were taken at the location mp-5. Wang et al. stated that the fluid flow is developed at this location and the experimental results obtained at this point.

Fig. 8-1 Thermocouple measuring points and the cross-section of the flow channel [206]

8.2.1 Power Distribution

Each fuel element in the fuel assembly generates heat, which is transferred to the coolant. Hence, the heat flux reflects the power generation distribution. In the idealized case, the heat flux along the axis would be uniform, however, in reality, it is affected by numerous phenomena ongoing in reactor and factors, i.e. moderation, fuel burn-up, variation in fuel enrichment, etc. In this chapter, the influence of these factors on a non-uniform heat flux along the axis direction is investigated.

Based on calculations of Tashakor et al. in 2013 [193], it is observed that the peak of power distribution is located upstream. Therefore, a user-defined function (UDF) file was prepared based on the equation used to predict the power distribution due to the variation of burn-up at different phases of life time [192]. The correlation of power distribution is shown in Chapter 6, Eq. 40.

Fig. 8-2 Normalized power distribution along the axis

A total of five cases were investigated and shown by the normalized power distribution in Fig. 8-2. The average heat flux value is the same in every case, with the only variables being the $N1$ and $N2$ coefficients in Eq. (40). Table 8-1 shows the values of each coefficient. The distribution in case 4 follows the trend presented by Tashakor et al. in their research paper.

Table 8-1 List of cases and change of variables in particular cases

Case No.	Variables
Case 1	N/A – uniform heat flux
Case 2	$N1 = 1, N2 = 1$
Case 3	$N1 = 3, N2 = 1$
Case 4	$N1 = 3, N2 = 1.3$
Case 5	$N1 = 3, N2 = 0.6$

8.2.2 Governing Equations

ANSYS Fluent like all CFD codes uses a number of governing equations to represent the fluid flow. The most important task is to solve the conservation equations of mass, momentum, and energy as described in the ANSYS Theory Guide [194] (see Chapter 3). In addition, turbulent flow must be considered. While different numerical turbulent models were created, no universal model was developed so far. Therefore, as a starting point, it is necessary to conduct a validation of different models against published experimental data. Based on earlier supercritical flow work of *Low-Reynolds Shear Stress Transport (SST) $k-\omega$* [207], the SST $k-\omega$ and the RNG $k-\varepsilon$ [216] turbulent models described in Chapter 3 were chosen for the calculations [87, 88].

8.2.3 Fluid Properties

Water properties at 25 MPa are similar to those shown in Fig. 7-1. The peak of the specific heat is at a temperature of 385°C or 658K. The “NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP)” contains properties information of many different fluids at sub- and supercritical conditions including water and it is incorporated in the ANSYS Fluent. The REFPROP version is 9.1.

Viscosity, density, and thermal conductivity swiftly decrease during the sub- to supercritical transition. The specific heat on the other hand, has a large peak at the critical temperature.

8.2.4 Geometry and Boundary Conditions

The supercritical water flows through a vertical 2x2 fuel assembly as shown in Fig. 8-1. The geometry used for computations is simplified to one fuel subchannel and symmetrical boundary conditions are applied on the side walls as it is shown in Fig. 8-3. The diameter of the fuel rod is 8mm, whereas the sides where symmetry condition is applied have 10.16mm, and the length of the fuel channel is 0.6m.

The simplification was made in order to save computational time and power without sacrificing the accuracy. Three meshes were generated for the independency study and their data can be found in Table 8-2.

Fig. 8-3 Scheme of the model

Table 8-2 Meshes used for independency study

Mesh	Perimeter	Axis	Radial	First wall (μm)	Number of nodes
#1	60	150	80	0.8	396000
#2	80	200	100	0.8	760000
#3	100	250	120	0.8	129000

After the validation study against data provided by Wang et al., 2014 [206], mesh #2 was chosen for further calculations due to its best accuracy among the others. The data found in Wang et al., 2014 shows the bulk temperature at 0.5m from the inlet, when three different inlet temperatures are applied, i.e. subcritical flow (217°C), during the transition from sub- to supercritical condition (381°C) and supercritical flow (415°C). Table 8-3 summarizes the mesh independency study. The following formula is used to calculate the error:

$$error = \frac{measured - actual}{actual} \cdot 100\% \quad (57)$$

Table 8-3 Mesh validation and error evaluation for different turbulent model

		Error at Different Inlet Temperatures			Average Error
Mesh summary		217°C	381°C	415°C	
Mesh #1	Low Reynolds SST $k-\omega$	-0.23%	0.28%	0.03%	0.18%
	SST $k-\omega$	-0.18%	0.28%	-0.02%	0.16%
	RNG $k-\epsilon$	-0.23%	0.27%	0.01%	0.17%
Mesh #2	Low Reynolds SST $k-\omega$	0.04%	0.29%	-0.01%	0.11%
	SST $k-\omega$	-0.16%	0.27%	0.08%	0.17%
	RNG $k-\epsilon$	-0.18%	0.27%	-0.03%	0.16%
Mesh #3	Low Reynolds SST $k-\omega$	-0.20%	-13.62%	-0.03%	4.62%
	SST $k-\omega$	-0.21%	0.27%	0.03%	0.17%
	RNG $k-\epsilon$	-0.19%	-13.63%	0.02%	4.61%

Moreover, the *Low Reynolds SST $k-\omega$* model has been found to be the most accurate with an error of 0.11% at measured point, i.e. 0.5 m from the inlet.

The boundary conditions at the operational pressure of 25 MPa are as follows: inlet temperature of 327°C, mass flux of 1000 kg/m² s and average heat flux of 600 kW/m².

8.2.5 Convergence Criteria

The convergence criteria used for the energy and continuity equation, velocity in x , y and z directions, turbulent kinetic energy and specific dissipation are all set to 10^{-5} . Cross-

sections at different distances from the inlet were monitored until they converged. In all cases, the outlet area-weighted average temperature is the same.

Following ASME CFD recommendations, all governing equations were solved with the use of second order differential schemes. Pressure-velocity was coupled with the use of SIMPLE scheme; the solver is pressure-based.

8.3 Results

The results presented in Figures 8-4 to 8-8 show temperature on the fuel rod wall in each calculated case. The legends below the figures explain at which particular angle location measurement was taken. The colours were adjusted to match the symmetry plane that goes through points at the 135° and 315° angle locations. However, not all cases give symmetrical results. The highest temperatures were observed at the gap region between fuel rods and an outer region of fuel subchannel, i.e. at angles of $22.5^\circ - 67.5^\circ$ and $202.5^\circ - 247.5^\circ$. Lower temperatures are close to the centreline, with the lowest temperature at the 315° angle location.

The wall temperature distribution along the axis is shown in Fig. 8-4. The heat transfer deterioration phenomenon (HTD) occurs when uniform heat flux is applied on the wall. At the upstream, a rapid temperature increase takes place. At some of the locations close to the inlet, the temperature rises close to the critical temperature, then decreases and again increases until the end of the channel. The maximum wall temperature of 420°C was reported at the outlet at two locations, i.e. 22.5° and 247.5° . It is possible to distinguish symmetry in the plot of wall temperatures.

The simplest sinusoidal heat flux distribution (case 2) has a noticeable influence on the wall temperature distribution (Fig. 8-5). The maximum wall temperature is higher than in reference case 1 with a value of 485°C at two locations, i.e. at an angle of 22.5° and 247.5° . The maximum temperatures occur at the gap region right after the middle of the fuel rod axis. This time the temperature increases only once. The most interesting part, in this case, is that the obtained results are the most symmetrical among all investigated cases.

Fig. 8-4 Wall temperature distribution along the axis position in case 1, uniform heat flux. Operating pressure is 25 MPa, the inlet temperature is 327°C, mass flux is 1000 kg/m² s and heat flux is 600 kW/m²

Fig. 8-5 Wall temperature distribution along the axis position in case 2, N1=1, N2=1. Operating pressure is 25 MPa, the inlet temperature is 327°C, mass flux is 1000 kg/m² s and heat flux is 600 kW/m²

Case 3 (Fig. 8-6) has a similar maximum value of heat flux as in case 2, however the peak of maximum wall temperature is moved upstream and the maximum is higher - 517°C at an angle location of 45°. It is nearly 100°C greater than when uniform heat flux is applied. The HTD occurs only at the gap between the fuel rods

Case 4 is the most interesting since the power distribution best matches the one predicted in a nuclear reactor by Tashakor et al. in 2012 [210] (Fig. 8-7). Similar to previous cases with non-uniform heat flux applied on the wall, HTD occurs. The wall temperature distribution is similar to case 3, however the maximum temperature is higher, i.e. 575°C, and located at the gap area between the fuel rods and outer part of subchannel, i.e. 45°. This case is characterized by the highest wall temperatures among all investigated cases.

The result of calculations when the power distribution curve has a lower peak and is rather uniform is presented in Fig. 8-8. Again, HTD occurs close to the inlet and the maximum wall temperature is 454°C at 225° angle location. It is lower than other non-uniform cases but exceeds the reference case.

Fig. 8-6 Wall temperature distribution along the axis position in case 3, N1=3, N2=1. Operating pressure is 25 MPa, the inlet temperature is 327°C, mass flux is 1000 kg/m² s and heat flux is 600 kW/m²

Fig. 8-7 Wall temperature distribution along the axis position in case 4, $N1=3$, $N2=1.3$. Operating pressure is 25 MPa, the inlet temperature is 327°C, mass flux is 1000 kg/m² s and heat flux is 600 kW/m²

Fig. 8-8 Wall temperature distribution along the axis position in case 5, $N1=3$, $N2=0.6$. Operating pressure is 25 MPa, the inlet temperature is 327°C, mass flux is 1000 kg/m² s and heat flux is 600 kW/m²

8.4 Discussion and Conclusions

Supercritical water flow in a 2×2 fuel rod bundle was successfully investigated with CFD software, and it provides better understanding of the phenomena ongoing while non-uniform heat flux was applied. Under supercritical conditions, the flow is very sensitive to changes of heat flux along the axis.

The results show Heat Transfer Deterioration (HTD) phenomenon occurs in all investigated cases. However, the higher the peak of heat flux, the higher is the maximum wall temperature. Case 4 (the most similar to predicted power distribution curve) is characterized by a 150°C higher maximum temperature than the reference case when the uniform heat flux is applied. The wall temperature is strongly correlated with the shape of power distribution curve along the axis and very sensitive to it.

When the peak in heat flux is located upstream, the maximum temperature drastically increases close to the fuel assembly inlet. Therefore, it is suggested to perform coupled CFD and neutronic calculations in order to predict how property changes will influence the temperature distribution during reactor operation. The rapid rise in temperature not only correlates with the changes of fluid properties because these, in turn, influence fuel moderation and power generation.

The rapid peaks of wall temperature occur only at the gaps between fuel rods, hence another interesting aspect for further investigation would be the use of wire wrapped fuel bundle instead of a bare bundle. This would increase fluid mixing, and potentially decrease the maximum wall temperature.

Chapter 9

Conclusions, Recommendations and Outlook

This chapter provides a brief conclusion of the results described in this thesis and makes some recommendations for future research. However, greater detail can be found in the conclusion section of each Chapter. The emphasis of this research was simulation of the thermal responses of the fuel assemblages in lead-cooled fast reactors and SuperCritical Water-cooled Reactors using a variety of geometries and with solid or annular fuel. Recommendations for future work consist of activities that could not be conducted at NTU or in Singapore due to restrictions of software availability and changes in the national nuclear power research agenda. The outlook considers the status of nuclear power internationally and how it may develop in the future.

9.1 Conclusions

The investigation of an innovative annular fuel design for lead-cooled fast reactors showed it has superior cooling capacity over the standard nuclear fuel (the centreline temperature is over 700°C lower than the reference solid fuel). This characteristic allows the uprating of power by 10% while meeting all safety parameters when a square fuel lattice is used. Moreover, it is possible to replace a reference fuel assembly with annular fuel of the same dimensions and geometry to achieve a similar or lower pressure drop along the fuel channel. On the other hand, the hexagonal fuel lattice also ensures superior cooling, however, it has a much higher pressure loss. Uprating of 10% in case of the hexagonal fuel lattice results in excessive coolant velocity, and is not recommended. The optimal design is a 18×18 square fuel matrix that can directly replace the reference solid fuel matrix and is characterized by a centreline temperature of 732°C (T_{ref} 1472°C) and a 128 kPa (p_{ref} 130 kPa) pressure drop.

Safety analysis of SuperCritical Water-cooled Reactors (SCWRs) found that ongoing work focuses on developing codes capable of conducting safety analyses of the various designs. Japan is most advanced in their SCWR designs, and successfully developed safety codes and conducted various accident scenario analyses for two designs of the Super Light Water cooled Reactor (Super LWR) and SuperCritical water Cooled Fast Reactor (SCFR). Other countries and research teams are at the stage of performing analyses of accident scenarios. Numerous experimental work using test loops have been made to optimize the fuel assembly.

Numerical investigations of supercritical carbon dioxide (CO_2) flow in a vertical tube under non-uniform heat flux led to the following conclusions. The comparison between experimental results when uniform heat flux was applied at the wall found that Swenson's formula provides the most accurate results and predicts places where heat transfer deterioration (HTD) can occur. When non-uniform heat flux is applied, Swenson's formula is accurate only to the point of HTD, and it tends to overestimate the downstream flow. For supercritical water flow Bishop's formula best simulated experimental results. Both coolants found HTD arises from large property changes in the coolant during the transition from sub- to supercritical flow. However, if the system is optimized, lower maximum temperatures are possible than when uniform heat flux is applied.

The investigation of supercritical water flow in a 2×2 rod bundle when non-uniform heat flux is applied concluded that any variation in the heat flux distribution leads to higher temperature. When the heat flux curve was most similar to the power distribution found during the literature review, the resulting maximum temperature is almost 200°C higher than when uniform heat flux is applied. The highest temperature is located at the gaps between the fuel rods.

9.2 Recommendations

The innovative annular fuel shows promising results from a heat removal perspective. However, further neutronic analyses are required to investigate the thermal response when more than one energy approximation is used, and include higher volumes of cladding material to better simulate the power distribution inside the core. The neutronic calculations are required to assure criticality of the reactor core for different materials configurations including fuel, cladding etc. Further optimization of the fuel elements and fuel assembly geometry is possible. It is recommended to perform studies where one or more inner channels are partially or fully blocked since the inner channels are rather small, hence the possibility of blockage is real. This study would evaluate if the maximum possible cladding temperature remains within the safety limits. Further evaluation of the mechanical properties is required to predict how annular fuel designs will respond to loads and stresses during operation and determine the strain limits. It would be interesting to include different fuel materials including UC or UN to further optimize the fuel element geometry and temperatures that incorporate thermohydraulics and neutronics analyses. Finally, it would be possible to use either sub-channel codes or CFD to obtain flow and temperature distributions inside the reactor core.

As previously noted, studies of supercritical flow should consider neutronics. Property changes during the transition from sub- to supercritical flow are enormous, where parameters such as density, thermal conductivity, specific heat, and viscosity are ca. 5-8 times lower than the values before the critical point. The main reason to couple the thermal and neutronic calculations is the rapid change of the density since this property influences moderation of the fuel. This evaluation would show real peaking factors in the reactor and provide a more accurate thermal response scenario. Investigation of how wire wraps and/or different channel geometries would influence the wall temperature could be the next step of research. It would provide information on those geometries most suitable

for SCWRs and deliver information for further optimization of the reactor concept. Simulations with different fuel assembly geometries and more fuel elements inside the fuel assembly would be the next step in evaluation. Comparison between square, hexagonal, and circular fuel lattices would identify the optimal geometry. To date, there is no universal heat transfer correlation valid both at sub- and supercritical conditions. It would be valuable to create a database of the heat transfer coefficient correlations and experimental results to find an appropriate formula for fuel rod calculations. Building a supercritical experimental loop that uses water (or some other fluid that has a lower critical point and applying scaling laws) as a working fluid would be essential to validate the simulation results. Through these experimental results, further improvement of the empirical relations for a supercritical fluid would be possible.

9.3 Outlook

Nuclear energy is at a turning point as a technology that can satisfy the ever-growing demand for energy and address global warming. On the other hand, public opinion is not convinced that this energy source is safe. All industries have promised that the emission of greenhouse gasses will be limited, and nuclear energy is one of the technologies that can significantly reduce emissions. The USA, Finland, China and the Russian Federation are planning to build new nuclear power plants, whereas countries such as Japan are conducting safety re-evaluations in order to ensure all safety requirements are satisfied and restart reactors soon. This technology is especially beneficial for base load power production. Recently, Small and Modular Reactors have attracted investment of \$452M from the US Department of Energy, and as the current thesis demonstrates novel fuel rod designs may offer larger margins in safety that can contribute to SMR implementation in distributed power grids with higher public acceptance.

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