TESIS DOCTORAL

METHODOLOGY FOR SPENT FUEL DRY CASK THERMAL-HYDRAULICS ANALYSIS FOR LONG TERM STORAGE

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Methodology for spent fuel dry cask thermal-hydraulics analysis for long term storage

Doctoral thesis

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Abstract

One of the largest challenges facing the nuclear industry is with the management of nuclear spent fuel. As the available space in the nuclear spent pools is shrinking, nuclear power plants have needed a temporal solution to storage the nuclear spent fuel before a more definitive or a country centralized solution is coming. This necessity has been met by using nuclear dry casks. This technology has been used for a long time but with the increase in burnout in the fuel and in the casks lifetime due to lack of progress in constructing central storage facilities has meant that more knowledge is needed regarding the behavior of the fuel during this part of its cycle.

In this sense, one of the key parameters is the Peak Cladding Temperature (PCT), which should not surpass 400 °C (USNRC, 2003). At that temperature, the hydrides dissolved in the clad can change their orientation and could cause embrittlement in the clads that could lead to rod failure. In order to ensure that this temperature limit is not surpassed, simulations are needed to verify it. These simulations can be done with Finite Elements (FE) codes such as Ansys Mechanical and with sub-channel codes such as COBRA SFS, but the most common way to simulate the dry cask thermal behavior is through Computational Fluid Dynamics (CFD) codes like Ansys Fluent, STAR-CCM+, CFX or OpenFoam, among others.

The main objective of this thesis is to create and validate a methodology that allows a CFD user to simulate a nuclear dry cask with enough accuracy and precision at a competitive computational cost. In order to do this, two different dry cask experiments were fully simulated. The first one was conducted by EPRI (The Electric Power Research Institute) in the 1980s using a real dry cask (called TN24P) and nuclear spent fuel. This first TN24P experiment served as the basis for the methodology, since the temperature distribution measured in the inner parts of the cask has allowed us to correctly develop the methodology. The simulations showed great accuracy and precision, with simulations agreeing with the experimental results, both on the outside and inside of the cask. Besides validating the results, different studies were performed to ensure that the CFD part of the methodology was done correctly, these included mesh independence studies using the Grid Convergence Index method, and turbulent modelling studies. Finally, another study was done to evaluate whether the gaps between the canister and basket had an impact on the thermal performance of the canister. This study showed that the size of these gaps was crucial, and they did have a large impact.

The second experiment used was performed by Sandia National Labs (SNL), and it consisted of a single dummy fuel assembly with electrical resistance to simulate the heat output of a real fuel assembly, in this case the fuel assembly was a BWR. The experiments were conducted at different pressures and heat outputs, which meant that the methodology could be tested at very different combinations of pressure and fuel power. This second experiment was used to test different ways to model the fuel assemblies including using porous media regions to test whether they were required to obtain good agreement to the experimental results. The way that CFD codes model porous media meant that the potential benefits of modelling these regions with porous media were outweighed by the negative effects they provided.

In the next part of the thesis, the methodology was taken beyond a single cask. The first of these works included simulating the drainage and drying process of the fuel cask. These processes showed that although possible to simulate these steps, the computing time was extremely high

meaning that many simplifications were required, and that further improvements may be required, either through a leap in computer capabilities, better simplifications or both.

The next study was checking whether a group of casks would impact the thermal performance to one another since casks are placed in storage facility near one another. Several configurations of 12 cask were tested, in all cases a single cask had better performance. The different configurations showed different levels of thermal impact, with some casks showing a significant increase in temperatures.

In the final part of the thesis the problem of the gap was tackle by coupling the results from the CFD code to a mechanical analysis, in this case ABAQUS. By coupling the results, the mechanical code could show thermal expansion of the different components shedding light to the behavior of the gaps. This study also was also used to see the thermal stress of the different components of the cask.

As a conclusion, the dry cask thermal methodology created was validated against different experimental tests and applied to several engineering realistic problems, showing its efficiency by combining precision with competitive computational cost.

Resumen

Uno de los retos a los que se enfrenta la industria nuclear es la gestión del combustible gastado, ya que el espacio disponible en las piscinas de combustible nuclear gastado desapareciéndose va reduciendo. Esta limitación en el espacio disponible ha supuesto que las plantas nucleares necesiten una solución temporal para almacenar el combustible gastado. Esta necesidad ha sido solucionada gracias al uso de contenedores de combustible nuclear gastado. Esta tecnología, aunque no es nueva, ha requerido aumentar los conocimientos de la respuesta del combustible gastado durante esta etapa de su ciclo debido al aumento del tiempo de operación de los contenedores.

En este sentido uno de los parámetros críticos es la temperatura máxima de varilla (PCT según sus siglas en inglés), la cual no debería superar los 400 °C (USNRC, 2003), temperatura a la cual los hidruros disueltos en la vaina cambian de orientación, lo cual puede causar fragilidad en las vainas y la rotura de las mismas. Para asegurar que este límite no es superado se necesita de simulaciones que corroboren que el comportamiento térmico del combustible es el adecuado. Estas simulaciones pueden llevarse a cabo con códigos de elementos finitos como Ansys Mechanical, con códigos de sub-canal como COBRA SFS o, la opción más común, mediante simulaciones de fluidos computacionales (CFD en sus siglas en inglés) con códigos como Ansys Fluent, STAR-CCM+ o OpenFoam entre otros.

El principal objetivo de esta tesis es crear y validar una metodología que permita a un usuario de CFD simular un contenedor de combustible nuclear gastado con precisión, exactitud y un coste computacional razonable. Para poder hacer esto, dos experimentos han sido simulados en detalle. El primero fue realizado por EPRI (The Electric Power Research Institute) en los años 80. El experimento hizo uso un contenedor de combustible con combustible nuclear gastado. Este experimento ha servido como la base de la metodología; gracias a los perfiles térmicos que se obtuvieron en el interior del contenedor los cuales permitieron el desarrollo correcto de gran parte de la metodología. Además de validar los resultados obtenidos también se llevaron a cabo una serie de estudios que permiten tener más fiabilidad en los resultados, como estudios de independencia de malla mediante el método de Grid Convergence Index y estudios de turbulencia. Otro de los estudios que se llevaron a cabo fue el estudio del tamaño de los huecos entre el bastidor y el cuerpo del contenedor y su impacto en la respuesta térmica del mismo. Este estudio demostró que el tamaño de los huecos tiene un elevado impacto en la respuesta térmica.

El segundo experimento fue realizado en los Laboratorios Nacionales de Sandia (EEUU), y consistió en un elemento combustible de tipo BWR construido con resistencias térmicas que permiten simular el calor residual de un elemento combustible real. Este experimento se realizó a diferentes presiones y potencias, lo cual permitió que la metodología fuese probada en diferentes condiciones. Este segundo experimento también se usó para probar distintas formas de modelar el combustible nuclear, por ejemplo, se probó a modelar las rejillas mediante medios porosos, y así comprobar si modelar estas regiones es necesario de cara a obtener resultados equivalentes a los de las simulaciones. En los resultados con STAR-CCM+, la forma en la que los códigos CFD modelan los medios porosos implicó que los posibles beneficios obtenidos de simular medios porosos no eran totalmente justificables con los problemas que estos introducían.

Las partes siguientes de la tesis buscan usar la metodología para casos de aplicación que van más allá de un contenedor en condiciones de almacenamiento estacionario. El primero de estos trabajos incluye la simulación de los procesos de secado y vaciado del contenedor. Estos procesos tan complejos requirieron muchas simplificaciones para mantener el coste computacional en unos niveles aceptables. A pesar de que se pudo simular parte de estos procesos los resultados demostraron que las simplificaciones tomadas no fueron las más adecuadas, por lo que, de cara a enfrentarse a este problema a futuro, se requeriría mejores simplificaciones y un salto en las capacidades computacionales.

El siguiente estudio lidia con averiguar si al poner un contenedor en condiciones de almacenamiento real (es decir junto a otros contenedores), la eficiencia térmica empeora. Para ello se probaron cuatro distribuciones de 12 contenedores. En todos los casos la eficiencia térmica empeoró con respecto al caso de un único contenedor, obteniéndose mayores temperaturas. El estudio también encontró que el impacto no era igual en todos los contenedores y que era más pronunciado en unos que en otros.

En la parte final de la tesis el problema de los huelgos se recupera, en este caso se usó los resultados obtenidos mediante CFD, y se acoplaron a un código de análisis mecánico, en este caso el código ABAQUS. Al acoplar los resultados se obtuvieron las dilataciones térmicas de los distintos componentes, lo cual permitió observar cómo evolucionarían los huelgos. A su vez también se pudo obtener los valores de las tensiones térmicas de los distintos componentes.

Como conclusión, la metodología para el cálculo de contenedores gastados fue creada y validada contra varios experimentos y aplicada a una serie de problemas de ingeniería, mostrando su eficacia, tanto en los resultados como en los costes computacionales.

Thesis Outcomes

Journal Articles Published (2)

- **Benavides, Julio**, Jimenez, G., Galbán, M., Lloret, M., 2019. Methodology for thermal analysis of spent nuclear fuel dry cask using CFD codes. Annals of Nuclear Energy 133, 257–274. <https://doi.org/10.1016/j.anucene.2019.05.026>. Q1 Journal Impact Factor 1.62
- **Benavides, J.**, Jiménez, G., López, S., Galbán, M., Lloret, M., 2020c. Modeling and results of the dry cask simulator (DCS) with STAR-CCM+. Nuclear Engineering and Design 369, 110820. <https://doi.org/10.1016/j.nucengdes.2020.110820>. . Q2 Journal Impact Factor 1.378

Journal Articles under review (2)

- **Benavides, Julio**, Costa Garrido, Oriol, Jiménez, G. Cizelj, Leon. Thermo-mechanical analysis of a nuclear spent fuel dry cask using CFD results in a FE code. Nuclear Engineering and Design (Uploaded October 2020).
- Andres Hernandez-Avellaneda, Gonzalo Jimenez, **Julio Benavides**, Luis Rey, Juan Carlos Martinez-Murillo. Nuclear spent fuel cask full scope simulation using coupled Computational Fluid Dynamics models. Nuclear Engineering and Design (Uploaded May 2020)

Conference papers (13)

- Ardura, A.A., Avellaneda, A.H., **Benavides, J.**, Varas, J., 2020. SIMULACIÓN DE UN ALMACÉN TEMPORAL INDIVIDUALIZADO GENÉRICO CON ANSYS CFX. Presented at the Reunión Anual Sociedad Nuclear Española 2020,
- Avellaneda, A.H., Rodríguez, **J. Benavides**., Varas, G.J., Rey, L., Martínez-Murillo, J.C., 2018. Estudio de un contenedor de combustible gastado mediante una simulación de geometría reducida empleando el código ANSYS CFX., in: Sociedad Nuclear Española. Presented at the Reunión Anual Sociedad Nuclear Española 2018.
- Barahona, M.G., Llorca, M.L., Rusiñol, C.S., Varas, G.J., **Benavides, J.**, 2017. Análisis de la temperatura del combustible durante el almacenamiento en seco y transporte., in: Sociedad Nuclear Española. Presented at the Reunión Anual Sociedad Nuclear Española 2017.
- Barahona, M.G., Llorca, M.L., Rusiñol, S., **Benavides, J.**, Jiménez, G., 2018. Estudio de sensibilidades del contenedor de almacenamiento de combustible gastado TN-24P con el código COBRA-SFS, in: Sociedad Nuclear Española. Presented at the Reunión Anual Sociedad Nuclear Española 2018.
- **Benavides, J.**, Costa Garrido, O., Jimenez, G., Cizelj, L., 2020a. ANÁLISIS TERMO-MECÁNICO DE UN CONTENEDOR DE COMBUSTIBLE NUCLEAR GASTADO. Presented at the Reunión Anual Sociedad Nuclear Española 2020, Online.
- **Benavides, J.**, Garrido, O.C., Jimenez, G., Cizelj, L., 2020b. Thermo-Mechanical Analysis of a Dry Storage System. Presented at the NENE 2020.
- **Benavides, J.**, Jimenez, G., Galbán, M., Lloret, M., 2018a. STAR-CCM+ SIMULATION OF A SPENT FUEL DRY CASK EXTERNAL COOLING BY NATURAL CONVECTION, in: TopFuel Prague September 2018. Presented at the TopFuel.

- **Benavides, J.**, Jiménez, G., Hernández-Avellaneda, A., Galbán, M., 2019. THERMAL STUDY OF SEVERAL SPENT FUEL CASK DISTRIBUTIONS IN A REPOSITORY USING CFD CODES, in: Proceedings ICONE27. Presented at the ICONE27.
- **Benavides, J.**, Varas, G.J., Barahona, M.G., Llorca, M.L., Rusiñol, C.S., 2018b. Estudio de los mecanismos de refrigeración del exterior del contenedor de combustible gastado TN-24P con STAR-CCM+, in: Sociedad Nuclear Española. Presented at the Reunión Anual Sociedad Nuclear Española 2018.
- **Benavides, J.**, Varas, G.J., Barahona, M.G., Llorca, M.L., Rusiñol, C.S., 2017. Estudio del contenedor de almacenamiento de combustible gastado TN- 24P con el código termohidráulico COBRA SFS., in: Sociedad Nuclear Española. Presented at the Reunión Anual Sociedad Nuclear Española 2017.
- **Benavides, J.**, Jimenez, G., Galbán, M., Lloret, M., 2019. Metodología de estudio térmico de un contenedor de combustible gastado con STAR-CCM+. Presented at the Reunión Anual Sociedad Nuclear Española 2019.
- Galbán, M., Lloret, M., **Benavides, J.**, Jiménez, G., 2018. TEMPERATURE CALCULATIONS IN SPENT NUCLEAR FUEL CASK USING COBRA-SFS, in: TopFuel Prague September 2018. Presented at the TopFuel.
- García, S.L., Rodríguez, **J. Benavides.**, Varas, G.J., 2020. Simulación de la inercia térmica del Uranio a partir de un material equivalente en las vainas de combustible gastado con STAR-CCM+. Presented at the Reunión Anual Sociedad Nuclear Española 2020.

International Reports (1)

- Modeling Validation Exercises Using the Dry Cask Simulator. Pulido, R.J.M., Lindgren, E.R., Durbin, S.G., Zigh, A., Solis, J., Suffield, S.R., Richmond, D.J., Fort, J.A., Herranz, L.E., Fera, F., Penalva, J., Lloret, M., Galbán, M., **Benavides, J.**, Jiménez, G., 2019. Spent Fuel and Waste Disposition 72.

Awards (2)

- Best Poster Award. for Thermo-Mechanical Analysis of a Dry Storage System. Presented at the NENE 2020, p. 8. **Benavides, J.**, Garrido, O.C., Jimenez, G., Cizelj, L., 2020b
- Student Best Poster at THE INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING presented at the 27th ICONE, Tsukuba, Ibaraki , Japan. **Benavides, J.**, Jiménez, G., Hernández-Avellaneda, A., Galbán, M., 2019. THERMAL STUDY OF SEVERAL SPENT FUEL CASK DISTRIBUTIONS IN A REPOSITORY USING CFD CODES, in: Proceedings ICONE27. Presented at the ICONE27.

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Contents

Abstract	I
Resumen.....	III
Thesis Outcomes	V
Agradecimientos	VII
Agradecimientos institucionales	VIII
Figures Index	XIII
Tables Index	XVII
Acronyms.....	XVIII
1 Motivation and thesis structure.....	1
2 Nuclear Spent fuel.....	3
2.1 Introduction to nuclear spent fuel	3
2.2 Spent fuel reprocessing.....	5
2.3 Transport.....	6
2.4 Long term storage	7
2.5 Dry cask systems	8
2.5.1 Dry cask loading	9
2.5.2 Doble Propósito Trillo.....	10
2.5.3 ENUN 32	11
2.5.4 TN-24P	12
2.5.5 HI-STORM	13
2.5.6 The Dry Cask Simulator (DCS).....	14
3 Computer Fluid Dynamics	17
3.1 Conservation equations	17
3.2 Turbulence	18
3.3 Turbulence models.....	20
1.1.1 Standard k- ϵ model	20
3.3.1 Two-layer approach	21
3.4 Convection and turbulence modelling.....	21
3.5 Porous media	22
4 Dry cask modeling state of the art	25
5 Methodology.....	29
5.1 Objectives and phases.....	29
5.2 Model creation and best practices.....	29
5.2.1 Geometry	29

5.2.2	Meshing.....	32
5.3	Core Methodology	35
5.3.1	Preliminary works.....	36
5.3.2	Fuel assemblies	37
5.3.3	COBRA SFS	40
5.3.4	Interior and exterior model.....	41
5.3.5	Grid Convergence Index	43
5.3.6	Turbulence modelling.....	44
5.4	Extended methodology	45
5.4.1	Drainage process	45
5.4.2	Temporal storage	45
5.4.3	Mechanical Calculation	46
5.5	Experiments.....	47
5.5.1	TN-24P	47
5.5.2	Dry Cask Simulator	53
6	Results	57
6.1	TN-24P	57
6.1.1	Numerical scheme, geometry, and boundary conditions	57
6.1.2	Grid Convergence Index	61
6.1.3	Turbulence modelling.....	64
6.1.4	Outside model results	66
6.1.5	Interior model results.....	69
6.1.6	New method of coupling the internal and external models	75
6.2	DCS	80
6.2.1	Geometry	80
6.2.2	Boundary conditions and numerical scheme	81
6.2.3	Turbulence modeling	82
6.2.4	GCI	83
6.2.5	Results	84
6.2.6	Conclusions.....	96
6.3	Drainage process.....	97
6.4	Storage facility.....	100
6.4.1	Study cases	101
6.4.2	Boundary conditions and numerical scheme	103
6.4.3	Results	103
6.4.4	Conclusions.....	108

6.5	Mechanical analysis.....	110
6.5.1	Structural model of the dry storage cask.....	110
6.5.2	Thermo-mechanical analysis results	116
6.5.3	Conclusions.....	122
7	Conclusions	123
7.1	Future works	125
8	References.....	127

Figures Index

Figure 1 Fission products of U^{235} (Serrano, 2001)	4
Figure 2 PWR fuel bundle decay heat as a function of time after discharge at 50 GWd/MTHM (Ade and Gauld, 2011)	4
Figure 3. The MP197HB shielded transport cask during training exercises at Waste Control Specialists (Image: Orano)Image: © Orano ("Orano-MP197HB-shielded-transport-cask," 2021).	6
Figure 4. Onkalo site (Posiva Oy, 2020).....	7
Figure 5.(a) Dry storage with bolted top, and (b) dry storage with welded top and an overpack (Greene et al., 2013, n.d.)	9
Figure 6. Loading of a nuclear dry cask ("Tipos de contenedores - CSN," 2008)	10
Figure 7. ENUN 32 (SEPI, 2019)	12
Figure 8. TN-24P (EPRI, 1987a).....	13
Figure 9. HI-STORM loading (CSN, 2011)	14
Figure 10. Dry Cask Simulator (Lindgren and Durbin, 2017a)	15
Figure 11. Fluctuating and mean variable components.....	19
Figure 12. Qualifications for the different models (Zhang et al., 2011).....	22
Figure 13. Channel description COBRA SFS.....	26
Figure 15. Neutron shield change	30
Figure 16. Preparing the fluid region	31
Figure 17. Errors during CAD import operation	32
Figure 18. Sweep or directed mesh.....	33
Figure 19. Badly mesh interface.....	34
Figure 14. Methodology diagram.....	35
Figure 20. DPT models, exterior model (left) and interior model (right) (Benavides, 2015).....	36
Figure 21. Temperatures inside the DPT (Benavides, 2015)	37
Figure 22. Streamlines of the upper plenum in the DPT (Benavides, 2015)	37
Figure 23. Real Fuel assembly (sketch) (US NRC, 2020a), an explicit fuel assembly and a porous media fuel assembly.....	38
Figure 24. Schematic thermal resistance for a system without clads (top) and with clads (bottom), on the right a simulation of a single assembly with and without clads.....	39
Figure 25. With and without clads inside the TN-24P, versus experimental results	40
Figure 26. Helium Flow in the TN-24P (velocities in mm/s). Blue is downward direction and red upward	41
Figure 27.Temperature (left) and heat transfer coefficient (right) on the neutron shield simulated versus calculated	42
Figure 28. Heat flux constant and directly mapped to the inner surface of the top lid	43
Figure 29. Interior storage facility (left (ENSA, 2014) and exterior facility (right (US NRC, 2020b)	46
Figure 30. Algorithm for coupling simulations, left as explained in the User's Manual of STAR-CCM+ (SIEMENS, 2018a) and right the developed methodology	47
Figure 31.Surry 15 x 15 PWR fuel assembly (side view left, cross section right)(EPRI, 1987b) ..	48
Figure 32. Predicted Axial Decay Heat Profile(EPRI, 1987b)	48
Figure 33. Spent fuel load pattern	49

Figure 34 Interior thermocouple locations(EPRI, 1987b).....	50
Figure 35. Exterior thermocouple locations (EPRI, 1987b)	50
Figure 36. Gated lower plenum (left) and approximation used for the TN-24P model (right)...	52
Figure 37 Laboratory.(EPRI, 1987b)	53
Figure 38. Aboveground configuration (left), belowground configuration (right) (Lindgren and Durbin, 2017c).....	54
Figure 39. DCS configurations and CYBL facility (Lindgren and Durbin, 2017c).....	54
Figure 40. DCS construction (canister and basket top four images, outside shell two bottom images)(Lindgren and Durbin, 2017c)	55
Figure 41. TC placements on the Fuel Assembly, Channel Box, Canister and Outside Vessel respectively (Durbin and Lindgren, 2017a)	55
Figure 42. Hot wire anemometer and honeycomb position (lefty), velocity profile calculated (right) (Durbin and Lindgren, 2017a)	56
Figure 43. Small room geometry.....	57
Figure 44. Interior model of the TN-24P	59
Figure 45. Heat output per assembly and distribution (EPRI, 1987c).....	60
Figure 46. Heat transfer coefficient on the neutron shield, heigth dependant value and 3-D distribution.....	60
Figure 47. Thermocouples in the inner part of the TN-24P (EPRI, 1987c).....	61
Figure 48. Exterior mesh	62
Figure 49. Fine mesh (left), Very FineXY mesh (right).....	63
Figure 50. Naming convention for the assemblies and periphery holes	63
Figure 51. Temperature profiles on the neutron shield (bottom left), the top lid (bottom right), and a schematic overview of where they have been extracted	65
Figure 52. Temperatures of the different turbulence models for the inner most assembly (bottom left), and outer assembly (bottom right).	66
Figure 53. Temperature on the TN-24P	67
Figure 54. Temperature on a plane.....	67
Figure 55. Temperature profiles at different depths (left), and concrete above 298 K	68
Figure 56. Temperature profile in a center line below the cask	68
Figure 57. Air temperature near the neutron shield and simulated heat transfer coefficient..	69
Figure 58. Gaps.....	70
Figure 59. Gap impact for different assemblies.....	71
Figure 60. Mass flow through the assemblies.....	72
Figure 61. Primary loop (left) and secondary loop (right).....	73
Figure 62. Mass flow through the periphery channels	73
Figure 63. Updraft velocity and downward velocity	74
Figure 64. Heat transfer throughout the canister, and radially	74
Figure 65. Temperature distribution, old method (left), latest method (right).....	76
Figure 66. Temperature distribution on the neutron shield (left) and on the top lid (right), on the old method and in the new one.....	76
Figure 67. Temperature on the concrete, old method (left), and new method (right)	77
Figure 68. Heat flux through the lower lid (New method).....	78
Figure 69. Temperature on the inner cask Wall old method (left), new method (right).....	78
Figure 70. Temperature on a middle height plane, old method (left), and new method (right)	79
Figure 71. Temperature distribution on the thermocouple lances in the different fuel assemblies. The red dot indicates roughly which guide tube was used.....	79
Figure 72. DCS geometry	81

Figure 73. Temperature difference between laminar and turbulent model	83
Figure 74. Mesh of the DCS.....	83
Figure 75. Temperature distributrion on the 100 kPa 5 kW (upper image) and 0.5 kW (lower image).....	84
Figure 76. PCT and axial level for the 0.5 kW experiments.....	86
Figure 77. Temperature profile 0.5 kW experiments.....	87
Figure 78. Velocity magnitude (m/s) 800 kPa 0.5 kW experiment for all 3 Cases	88
Figure 79. PCT and axial position for the 5 kW experiments and simulations.....	89
Figure 80. Temperature distribution along the axial length	90
Figure 81. Temperature with (Case 2) and without spacers (Case 1)	92
Figure 82. Axial temperature profile for Cases 2B and 3B	93
Figure 83. Axial temperature profile in Case 3B	94
Figure 84. Boundary conduction heat flux upper channel box (100 kPa 0.5 kW).....	95
Figure 85. ENUN 32 Exterior and interior models (Benavides, 2016).....	97
Figure 86. Fraction of water at 3.4 seconds in the cask (left), and water flow direction during drainage (right)(Benavides, 2016).....	98
Figure 87. Flow direction change in the drainage tube (Benavides, 2016).....	99
Figure 88. Water volume fraction (top images) and fuel temperatures (bottom) at 54 seconds (left) and 120seconds (right) (Benavides, 2016)	99
Figure 89. Water fraction and temperature in one assembly at 120 seconds (Benavides, 2016)	100
Figure 90. Interim facility CNT (ENSA, 2014).....	101
Figure 91. The four distributions used	102
Figure 92. Cask numbering sequence	102
Figure 93. Temperature on the surface of a single cask	104
Figure 94. Maximum temperatures (normalized).....	105
Figure 95. Surface weighted average temperatures (normalized)	105
Figure 96. Surface weighted average HTC (normalized)	106
Figure 97. Percentage of radiation.....	106
Figure 98. Temperatures on Case D	107
Figure 99. Temperatures on Case A	107
Figure 100. Tracelines on Case D	108
Figure 101. Radiation heat flux cask 11 and cask 12 Case D.....	108
Figure 102. Geometry of the ¼ model of the cask and its components in the structural model in ABAQUS.....	111
Figure 103. Finite element meshes of the cask's components. Note that a short vertical section of the fuel pin assembly was shown here	112
Figure 104. Mechanical boundary conditions on the cask's components.....	113
Figure 105. Temperature distribution of the complete cask without fuel assemblies.....	114
Figure 106. Temperature distributions mapped onto the FE meshes of the (a) top lid, (b) bottom lid, (c) neutron shield and (d) steel canister with neutron shield.....	114
Figure 107. Temperature distribution of the basket.....	115
Figure 108. Temperature of the fuel bundle of assemblies, of a single fuel assembly from the periphery and of a short section of a single rod cladding.....	116
Figure 109. Displacements magnitude (left) and radial component (right) of the canister and neutron shield	116

Figure 110. Von Mises stress distribution in the canister and neutron shield (a and b – deformation scale factor 700), in the canister without neutron shield (c) and stresses along a circumferential path at middle height of the inner surface of the canister (inset graph).....	117
Figure 111. Displacements in the axial (left) and radial (right) directions of the basket.....	118
Figure 112. Von Mises stress distribution in the basket and the stresses along the centerline (inset graph)	118
Figure 113. Displacements magnitude of the fuel bundle of assemblies and of two individual assemblies: central (right) and periphery (left). Note the deformation scale factor of individual assemblies and that these have been rotated 90 around z-axis with respect to the fuel bundle	119
Figure 114. Von Mises stress distribution in the fuel assemblies	119
Figure 115. Temperatures of the central assembly obtained in three CFD simulations using different thermal resistances to model the gaps versus the experimental results (Benavides et al., 2019).....	120
Figure 116. Relative displacements along height between the basket and canister at the C1 (left) and C2 (right) gap locations (see Figure 57).....	121

Tables Index

Table 1-1. Total spent fuel status per region in (t HM) (IAEA, 2018a)	5
Table 1-2. . Commercial scale reprocessing facilities (IAEA, 2018a)	6
Table 1-3. Dry casks systems modeled in the thesis	9
Table 1-4. Fuel types for the ENUN32 cask (Equipos Nucleares, SA (ENSA), 2015).....	12
Table 1-5. Fuel requirements for the HI-STORM (CSN, 2011).....	14
Table 3-1. Summary of modeling (Pulido et al., 2019a).....	27
Table 6-1. Results for the small room and the large room	58
Table 6-2. Physical and numerical scheme	58
Table 6-3. Heat output distribution	59
Table 6-4. Exterior meshses	61
Table 6-5. GCI exterior model	62
Table 6-6. Inner meshes	62
Table 6-7. GCI inner simulation.....	63
Table 6-8. Nusselt number	65
Table 6-9. PCT for the different gaps	70
Table 6-10. Numerical and physical scheme	82
Table 6-11. Number of cells in each mesh	84
Table 6-12. GCI results	84
Table 6-13. Experiments.....	85
Table 6-14. Cases reference	85
Table 6-15. Air mass flow	88
Table 6-16. Air mass flow	91
Table 6-17. Heat transder mechanism 0.5 kW 100 kPa (%).....	95
Table 6-18. Heat transfer mechanism 0.5 kW 800 kPa (%).....	95
Table 6-19. Heat transfer mechanism 5 kW 100 kPa (%).....	96
Table 6-20. Heat transfer mechanism 5kW 800 kPa (%).....	96
Table 6-21. Physical and numerical scheme	103
Table 6-22. Results for a single cask.....	104
Table 6-23. Material properties of the cask's components	111
Table 6-24. Number of elements in components' meshes	112
Table 6-25. Maximum and average relative displacements between basket and canister.....	122

Acronyms

ν	Kinematic viscosity
v	Velocity
χ	Porosity
μ	Dynamic viscosity
μ_t	Turbulent viscosity
A_f	Face area
BT	Bolted top
BWR	Boiling Water Reactor
CFD	Computational Fluid Dynamics
CIEMAT	Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas
C_p	Heat capacity at constant pressure
DCS	Dry Cask Simulator
DPT	Doble Purpose Trillo
E	Energy or total energy per unit mass (e)
ENSA	Equipos Nucleares S.A.
EPRI	The Electric Power Research Institute
f_b	Force resultant of the body forces
FE	Finite Elements
GCI	Grid Convergence Index
h	Grid size or heat transfer coefficient
H	Enthalpy
INEL	Idaho National Engineering Laboratory
k	Kinetic energy or thermal conductivity
Kg	Kilogram
kt	Thermal diffusivity
kW	Kilowatt
KWU	Kraftwerk Union
L	Characteristic Length
ℓ	Length scales

MTU	Mega Ton of Uranium
MWd/tU	MegaWatts day per ton of Uranium
NRC	Nuclear Regulatory Commission
PCT	Peak Cladding Temperature
Pi	Inertial resistance tensor
PNNL	Pacific Northwest Laboratory
Pv	Viscous resistance tensor
PWR	Pressurize Water Reactor
q	Heat flux
r	Grid refinement ratio
SA	Surface weighted average
SE	Energy source per unit volume.
SNL	Sandia National Laboratory
UPM	Universidad Politécnica de Madrid
WT	Welded top
β	Coefficient of thermal expansion
ε	Dissipation rate
ρ	Density
σ	Stress tensor
φ_f	Face value of the scalar

1 Motivation and thesis structure

This PhD started as a part of a bachelor degree work, like many do, due to my interest in CFD and nuclear energy. The first steps was to learn CFD, a duty that it still a work in progress and will probably continue for as long as I continue to work with these tools. That first work not only served as a learning experience, but also as a starting point of this thesis. Many hypotheses were used in that work that could not be at that time due to lack of knowledge and data and although many of the assumptions made have been proven wrong, others have proven to be successful.

As will be discussed later, there is a need to understand the behavior of nuclear spent fuel during its dry storage phase in many countries, Spain among them. This need was boosted by the fact that the centralized storage facility in Spain was being delayed and the space left on the nuclear spent pools was running out. This necessity was the main motivator behind the drive of these works, having the goal to understand the thermal response of this systems and therefore to develop a methodology to calculate this response.

The first few chapters are an introduction to nuclear spent fuel and its life cycle. The latter chapters of this introduction into the fuel cycle, deal with the dry storage phase, describing the loading and drying of the fuel inside a cask, and describing the cask itself. Five different cask will be describe, of those three are commercial cask being used nowadays, the other two cask were built for experiments, with the TN-24P holding real nuclear spent fuel, and the DCS holding an electrically heated dummy fuel.

After the casks have been introduced, the main tool used to calculate the thermal response will be presented. CFD codes are complex, and the theory and techniques behind them mean that only an introduction will be feasible. After this, the main turbulent models that have been employed will be explained. Finally the last part of the introduction will explore how CFD codes have been used to simulate casks in the past, and what is available in the scientific literature.

The second part of this work is to show the methodology and how it was developed. This section will include some guidelines regarding model creation, meshing and other tips that may help future users. In this chapter the different steps needed for the correct application of the methodology will be detailed. The extended methodology, which include those works that go beyond a thermal calculation of a single cask in storage will de detailed here. These works include the draining process, the thermal performance of casks when they are placed in a storage facility and finally a mechanical analysis of a dry cask. This chapter will also explain the two different experiments, their set up and some of the limitations that were found when reviewing the available data.

Finally, the third chapter deals with the results of the methodology. This includes all the steps that were outlined in previous chapters, like turbulence modelling studies, the mesh independence studies and others such as the gap size of whether modelling the spacer grid are required. These sections are the core of this work and of the methodology, as they show the validation process and limits of what the methodology can accomplish.

The last chapter will deal with the conclusions of the thesis and future works.

2 Nuclear Spent fuel

In this chapter, a brief overlook at the different strategies of spent fuel management will be presented. First, what is nuclear spent fuel and why a safe storage solution is necessary, how much nuclear spent fuel there is in the world and how different countries have different policies regarding nuclear spent fuel (whether open or closed cycle). Finally, the last part of this chapter will introduce nuclear spent fuel dry cask systems: what they are, the different types of dry cask systems, how they are loaded with the spent fuel and how they are stored.

2.1 Introduction to nuclear spent fuel

Radioactive waste is a byproduct of nuclear power generation and other uses of radioactive material (medical, industrial or research). The radioactive waste can be solid, liquid, or gaseous with different radioactivity levels and half-life. In all cases, it must be handled safely and according to the preferences and practices of the different countries.

It is worth noting that the IAEA report on the spent fuel ("Joint Convention on the Safety of Spent Fuel Management and on the Safety of Radioactive Waste Management," 2009) is the only international legally binding instrument on this type of waste (spent fuel). Article 1 of this convention states:

"The objectives of this Convention are:

1. to achieve and maintain a high level of safety worldwide in spent fuel and radioactive waste management, through the enhancement of national measures and international co-operation, including where appropriate, safety-related technical co-operation;
2. to ensure that during all stages of spent fuel and radioactive waste management there are effective defenses against potential hazards so that individuals, society and the environment are protected from harmful effects of ionizing radiation, now and in the future, in such a way that the needs and aspirations of the present generation are met without compromising the ability of future generations to meet their needs and aspirations;
3. to prevent accidents with radiological consequences and to mitigate their consequences should they occur during any stage of spent fuel or radioactive waste management."

Each specific country which has high activity nuclear waste such as the spent fuel has their specific legislation which complements the IAEA safety standards.

The spent fuel radioactivity comes mainly from the operation of the reactor. When a uranium nuclei (U-235 or U-238) suffers fission, it can produce up to 600 different nuclei with different probabilities, for example in Figure 1 the fission products of uranium 235 (X axis is chain mass, and Y fission yields per 100 fissions). This initial chain kick starts the decay chain for the fission products that will last for thousands of years in some cases.

Figure 1 Fission products of U^{235} (Serrano, 2001)

These nuclei are rarely stable and have high radioactivity levels, which are high enough to generate significant quantities of heat due to the decay process in the first stage. As an example, in Figure 2 it can be seen the decay heat from a PWR fuel bundle for both MOX fuel and UOX from discharge to the first 10000 days (27 years).

Figure 2 PWR fuel bundle decay heat as a function of time after discharge at 50 GWd/MTHM (Ade and Gauld, 2011)

There is an estimated 250000 t HM (tonnes of heavy metal) of spent fuel in storage worldwide and 120000 t HM of reprocessed fuel (data from December 2013, accounting for 95% of nuclear

power reactors in the world,(IAEA, 2018a)). As for the total solid inventory radioactive waste is approximately 35 million m³, of which 28.5 million m³, has been disposed permanently and a further 6.3 million m³ is in storage awaiting final disposal (December 2013, (IAEA, 2018a)). Of this solid waste, 98% (in volume terms) is classified as being very low or low-level waste. In terms of total radioactivity, the situation is reversed with approximately 98% of the radioactivity being associated with intermediate and high-level waste.

Table 2-1. Total spent fuel status per region in (t HM) (IAEA, 2018a)

	Wet storage	Dry Storage	Reprocessed	Total
Africa	850	50	n.a. ^a	900
Eastern Europe	28600	2700	3200	40000
Western Europe	37000	4600	108400	154100
Far East	32100	5700	8600	46400
North America	79300	41900	n.a. ^a	121200
Latin America	3000	2000	n.a. ^a	5000
Middle East and South Asia	n.a. ^a	n.a. ^a	n.a. ^a	n.a. ^a
South East Asia and Pacific	n.a. ^a	n.a. ^a	n.a. ^a	n.a. ^a
Global total	180800	56900	120300	367600
Joint Convention Contracting Parties	177000	56900	120300	363700
EU Member States ^b	43300	6800	107600	162300
OECD/NEA members	166100	53200	119900	343800
	Possible differences in totals are due to rounding. In some regions no specification was made between wet and dry storage			
a	not applicable (or none reported)			
b	Excludes Austria, Greece, Malta and the Netherlands			

2.2 Spent fuel reprocessing

Spent fuel is generated when operating nuclear fuel in commercial and experimental reactors. In some countries, the spent fuel is considered directly as waste and it is disposed after three operational cycles. In other countries, it is considered a potential energy resource which can be reprocessed to recover fissile materials and to create Mixed Oxide (MOX) fuel. While most countries have adopted direct disposal of spent fuel, several countries have a reprocessing policy. These countries have large nuclear programs (France, China, the Russian Federation, and the United Kingdom). The case of Germany, Japan, Spain, and the United States of America is quite singular: they have changed from reprocessing and recycling as the first strategy to direct disposal. In Table 2-2 commercially scaled reprocessing facilities are shown.

The uranium separated during the reprocessing phase can be used in current reactors, if necessary, it could be enriched, whereas the plutonium can be used to create MOX fuel, as of 2018 only France has a commercial MOX fuel fabrication facility in operation (it provides services to several other countries).

Table 2-2. . Commercial scale reprocessing facilities (IAEA, 2018a)

Country	Facility	Capacity (t HM/a)	Status
France	UP2-400, La Hague	400	Under decommissioning
	UP2-800, La Hague	800	In operation
	UP3, Marcoules	800	In operation
	UP1, Marcoule	600	Under decommissioning
Japan	Rokkasho	800	Under commissioning
Russian Federation	RT-1, Mayak	400	In operation
	RT-2, Zheleznogorsk	60	Under decommissioning
United Kingdom	NDA THRP, Sellafield	900	In operation
	NDA Magnox Reprocessing	1500	In operation

2.3 Transport

No matter the policy regarding spent fuel, sooner or later fuel management involves a transport stage, whether is from the plant to the reprocessing site, or from the plant to the repository site. Transport is undertaken in designed transport containers that provide security, shielding and can keep the fuel cool. The transport is strictly controlled by national regulations. When the fuel has to cross national boundaries, each country has to take the appropriate steps to ensure that the transport is performed in an appropriate manner with the approval of all the countries involved. Most countries regulations are based on the IAEA Safety Standard “Regulations for the Safe Transport of Radioactive Material” (IAEA, 2018b).

Figure 3. The MP197HB shielded transport cask during training exercises at Waste Control Specialists (Image: Orano)Image: © Orano (“Orano-MP197HB-shielded-transport-cask,” 2021).

2.4 Long term storage

The first step of the nuclear fuel management is the pool storage, as it is an adequate way of keeping it cool while maintaining the workers and the environment safe. Since it was a necessary component most nuclear reactors have large storage pools in site in a separate building. The exception are the KWU reactors, like Trillo NPP, which has smaller pools inside the containment building. Due to increased lifespan of some reactors, the limited space in the pool (especially for KWU reactors) and the fact that centralized storage facilities have not been built yet in many countries (like Spain), a considerable number of nuclear power plants have built in house storage facilities using dry or vault systems. In latter chapters a more in depth look at dry cask systems will be presented.

As a different situation, High Level Waste (HLW) from reprocessing is typically vitrified and then it can be disposed directly in a deep geological repository at depths of several hundred meters (typically 500 m). Geological disposal facilities for long lived waste, can provide passive, multibarrier isolation of radiation materials if properly constructed and managed.

These emplacements sites should be placed in a tectonically stable region, where processes that could disrupt the disposal facility are slow or inexistent. Deep rock and underground water must remain stable for hundreds of thousands or even millions of years. Nonetheless, the spent fuel will be encapsulated in a corrosion resistant and mechanically stable container, covered by expansive clays, such as bentonite.

As of 2020 there are no active operating geological repositories, nonetheless the ONKALO underground research facility in Finland is near completion and should begin operations in 2023. Sweden and France are close to the construction and implementation of their own. In the United States of America, the license for the repository on Yucca Mountain Nevada has gone through several stages including a completed safety review evaluation by the NRC (Nuclear Regulatory Commission) in 2015, nonetheless it seems that the repository will not be operated, as founding and political support for the facility has dwindle. Germany has explored the option of using salt beds in Gorleben, but the work was suspended in 2013, and new emplacement sites are being explored. France has plans to start developing the design on the project Cigeo in clay host rock, with the expectation of starting operation in 2025 (IAEA, 2018a).

Figure 4. Onkalo site (Posiva Oy, 2020)

2.5 Dry cask systems

Since most centralized storage emplacements are not in operation yet, the need to storage spent fuel outside the nuclear spent pool has greatly increased. To solve this challenge most nuclear facilities operators have turn to dry cask systems, although initially though only as a way to storage the spent fuel for a few years until centralized storage facilities were opened, now the dry cask systems are starting to become a longer term solution (up to 50 years instead of the 20 years of initial design time).

In this sub-chapter, the two main types of dry cask systems that have been widely used in the industry will be explained and briefly compared:

- The dry storage system with Bolted Top (BT) which sometimes can be used for both storage and transportation (Figure 1a).
- The dry storage with Welded Top (WT) with an over pack (Figure 5b). For the WT, three overpacks are needed, one for transference (inside the facilities), one for transportation (between facilities) and one for storage (Figure 5 shows a concrete overpack for storage).

Throughout the work presented in this thesis both types of casks have been analysed, therefore both systems will be introduced in this chapter. The casks that were modelled or worked on throughout this thesis are summarize in Table 2-3.

Since most cask have similar components and work in a similar fashion, the general components, and how they work are summarized:

- Main body: made of stainless steel around 5 meters tall, the diameter varies depending on the number of fuel assemblies (and type it can hold). The main body is usually made of a single layer of steel. BT casks have a hollow exterior ring in which neutron absorbing material is located. To help dissipate the heat, copper or aluminium fins are place radially in the ring. WT casks do not have the neutron shield since they employed an overpack.
- The inner cavity of the casks is closed by an inner lid, this lid has penetrations to drain and fill the cask, and in the case of BT it sometimes has other penetrations to measure the inner pressure. On top of this lid some BT casks have a pressurized chamber filled with helium at high pressure, this helps detect any potential leakage from the inner cavity. Over the inner lid, an intermediate lid is placed to protect the inner lid (if it has the pressurized chamber, it also seals it). Finally, an outer lid with neutron absorbing material is placed on top, to lower the radiation to the outside. The lid for a WT is significantly simpler with only one lid that has a drain and a fill hole.
- In the inner cavity of the cask, the basket holds the fuel assemblies. The basket is a structure with squared tubes that separates the different fuel assemblies. The main structure is usually made of steel. To prevent criticality accidents some neutron absorbing material (in many cases borated aluminium) is placed between the fuel assemblies. Besides the basket, in the inner cavity there are other structural components: the drain tube and, in some cases, aluminium disks to help dissipate the heat.

Due to proprietary nature of many of the components, and the drawings necessary to build the models the descriptions and images will be mostly based on public records. The two casks used for experiments, the DCS and the TN-24P, have significantly more public

information (both in terms of the cask itself and the inner temperatures), making them the perfect casks for creating a methodology.

Table 2-3. Dry casks systems modeled in the thesis

Cask Name	Manufacturer	Use	Type
Doble Propósito Trillo (DPT)	ENSA	Commercial	BT
Enun 32	ENSA	Commercial	BT
TN-24P	Transnuclear Inc	Scientific Testing	BT
DCS	Sandia National Labs for the Extended Storage Collaboration Program (ESCP)	Scientific Testing	WT
HI STORM 100	Holtec International	Commercial	WT

Figure 5.(a) Dry storage with bolted top, and (b) dry storage with welded top and an overpack (Greene et al., 2013, n.d.)

2.5.1 Dry cask loading

In this section, a brief description on how a dry cask is loaded will be presented. This section is based in the working knowledge on how certain nuclear power plants in Spain load their casks and how the drain process takes place. Unfortunately this process is not very detailed in the publicly available literature, nonetheless a summarize can be found on this section (U.S.NRC, 2010). Since this information is proprietary the descriptions that follow are brief and generic on purpose.

The first step is to choose those fuel assemblies that are in compliance with the safety limits of the cask and the Regulatory Body criteria. The characteristics evaluated in each fuel assembly are heat decay, maximum burnup, time spent in the spent fuel pool, maximum initial enrichment

and whether the fuel assemblies are intact or not (some casks are only licensed for intact fuel assemblies, damaged assemblies need further encapsulation before being placed in a cask).

The second step consist of placing the cask in the spent pool, Figure 6, since handling spent fuel assemblies have to be done always under water for shielding the workers and make sure a proper cooling of the fuel assemblies. After the pre-selected assemblies are loaded, the inner lid is placed and the cask is extracted from the pool, full of water.

After this, the draining and drying take place, in this process the temperatures are closely limited, to prevent reaching 400 °C of PCT (Peak Cladding Temperature) (for burnups higher than 45 GWd/MTU). The fill hole is connected to a compressor that pushes air or nitrogen at high pressure into the cask so that the water is drained through the drain hole. Once no water is detected in the drainage hose, the process changes to nitrogen. With the valves at the entrance and exit line close, the nitrogen is left at atmospheric pressure for several minutes. Then the valves are open, and nitrogen is circulated at slightly higher pressures for several minutes. After this, the valves are closed again. This operation is repeated for several hours, in each step the water in the cask is reduced.

The final step before filling the cask with helium is to generate a vacuum inside the cask for a few minutes or until the pressure reaches a threshold (initially, if done properly this pressure should decrease in each cycle). Then the filling valve is open, and nitrogen is introduced. After a while, the valve in the drainage line is open for a period or until the inner pressure is low enough. This process is cycle until a can be reached, and hold for some time, when this happens, the cask is assumed dry and the helium is pumped into the cask. Overall, this proceeding should not take longer than 48 hours.

Figure 6. Loading of a nuclear dry cask ("Tipos de contenedores - CSN," 2008)

2.5.2 Doble Propósito Trillo

The Doble Propósito Trillo (Doble Purpose Trillo or DPT) is a cask design and manufacture by ENSA. The name indicates that it has a doble purpose, in this case the design allows for both transportation and storage. The initial helium pressure inside the cask is 1 atmosphere.

The DPT is licensed for the following requirements (CSN, 2013; Martínez, 2002):

- Hold up to 21 undamaged KWU 16-16 elements.

-
- Maximum initial mass of uranium of 480 kg per fuel bundle.
 - Maximum average burnup per element of 40.000 MWd/tU.
 - Minimum cooling time in the spent fuel pool of 5 years.
 - Maximum decay heat per element of 1,16 kW (24,35 kW whole cask).
 - Maximum initial enrichment of 4% in weight of uranium 235.

The DPT is a multi-wall cylinder 5 meters tall and 2.3 meters of diameter approximately. The cask is made of the following components:

- A vase made of several cylindrical pieces made of stainless steel and lead (to block gamma radiation) and a “floor”. The base has also an empty polygonal ring in the exterior, that is filled with neutron absorbing material and with radial copper fins to help dissipate the thermal heat. The floor is also made of two pieces of steel separated by a neutron absorbing material.
- The two lids made of steel. The inner lid has several penetrations to monitor the pressure of the inside of the cask and to drain and fill the cask. The outer lid is to protect the inner lid. On top of the outer lid another is placed with neutron absorbing material to help reduce radiation levels.
- Steel trunnions so that the cask can be move with a crane.
- The inner cask is composed of steel squared tubes to hold the fuel assemblies, surrounding the tubes there is a matrix of borated aluminum to both absorb neutrons and to help dissipate the heat. The inside part of the cask also holds steel disks for structural integrity and aluminum disk to dissipate heat. The inside also has the drain tube.

2.5.3 ENUN 32

The ENUN 32 is a cask design and manufacture by ENSA (Equipos Nucleares SA) . Like in the DPT case this cask can be used both for storage and transportation. It can hold up to 32 undamaged PWR fuel assemblies for up to 50 years, as is shown in the public report to the CSN (Equipos Nucleares, SA (ENSA), 2015). The initial helium pressure inside the cask is 1 atmosphere. It is licensed to hold two different types of fuel assemblies 16x16 KWU and a Westinghouse 17x17, each type has slightly different requirements as can be seen in Table 2-4. The cask has three different ways in which the load can be distributed:

- Uniform load: maximum load per assembly of up to 1.1 kW, therefore a maximum of 35.2 kW for the whole cask.
- Region-based load: two differentiated regions, in the 12 inner elements the maximum load is of up to 1.35 kW, and the 20 outside elements with maximum load of up to 1 kW, therefore the maximum for the whole cask is 36.2 kW
- Load with non-fuel hardware: the four central spaces are reserved for non-fuel elements such as control rods, primary or secondary sources or consumable neutron poison, their activity has to be limited to $2 \cdot 10^5$ Ci. The rest of the 28 positions can hold fuel assemblies with a maximum load of 1.1 kW per assembly for a total for the whole cask of 35.2 kW.

The cask is cylindrical in shape with a diameter of 2.6 meters and a height of 4.8 meters, the components in the cask are fairly like those of the DPT:

- The main body of the cask is made of low alloy carbon steel, where the different parts are welded together.

- The neutron shield is made of a neutron-absorbing resin that is poured in the spaces between the aluminium fins (to help dissipate the heat). The neutron shield is then surrounded with steel to protect the components from the environment.
- The cask has two lids, both lids are bolted down.
- The interior basket is made of steel and a neutron absorbing material called Metal Matrix Composite.
- Finally, the trunnions on the outside to help move the cask.

Table 2-4. Fuel types for the ENUN32 cask (Equipos Nucleares, SA (ENSA), 2015)

Fuel type	KWU 16x16	Westinghouse 17x17
Burnup range (MWd/MtU)	15.000 to 65.000	15.000 to 65.001
Enrichment range (in Uranium 235)	1.9 to 4.9%	1.9 to 4.9%
Time in spent in the spent pool (years=	3 to 18	3 to 22.5

Figure 7. ENUN 32 (SEPI, 2019)

2.5.4 TN-24P

The TN-24P was a cask that was design and manufacture by Transnuclear Inc. The cask is around 5 meters tall, 2.2 meters in diameter, and weighting 75 tons when empty, and 102 tons when fully loaded. In the 1980s EPRI (Electric Power Research Institute) conducted a series of experiments with it (EPRI, 1987a). In those experiments, the cask was loaded with 24 15x15 PWR fuel assemblies with a maximum heat output registered during the experiments of 20.6 kW.

The experiments consisted in measuring the temperatures in the cask under different positions (vertical and horizontal), and with the cask filled with nitrogen, helium and under a vacuum. The temperatures were measured using thermocouples that were introduced with lances from the top of the cask, this way the temperatures obtained had both an axial and a radial profile. The initial helium pressure inside the cask is 1 bar. Figure 8 a cut view of the cask is shown, the cask had the following components:

- The main body of the cask is made of stainless steel
- The inner cask has the basket made of borated aluminum and the drain tube.
- The neutron shield is a composite, made of radial copper fins, to help dissipate the heat load, and a neutron-absorbing resin. The neutron shield is covered by stainless steel to protect the different components from the environment

- The top of the cask is closed with two bolted lids, for the experiments only the interior lid was bolted. The interior lid had several penetrations so that the thermal lances could be inserted.
- Finally, the trunnions are placed in the cask so that it can be moved.

Figure 8. TN-24P (EPRI, 1987a)

2.5.5 HI-STORM

The HI-STORM cask is design and manufacture by Holtec International. Unlike the previous casks, the HI STORM is a WT system instead of a BT system, this is not the only difference: the HI-STORM works at higher inner pressures around 6 bar. Another difference is that the cask itself the MPC (multi-purpose cask) is inserted into different overpacks depending on the need. There are two transport overpacks the HI-TRACK and the HI-STAR, and one for storage the HI-STORM. To move it across the facility the HI-TRAC is placed on top of the MPC, it consists of a lead, steel and water cover, this over pack is meant to be used when moving the cask from the nuclear spent pool to the storage facility inside the NPP. The storage overpack is called HI-STORM and is made of concrete, steel, and lead, with air ducts from the outside to the inside to help dissipate the heat. Finally, the transport overpack is called HI-STAR and is made up of three shells, the first one that acts as the containment boundary, a series of steel shells, and a shell that houses neutron shielding material (CSN, 2011).

The MPC is relatively simple compared to the previous casks, its main body is made of stainless steel and it is closed by welding the lid. Inside the cask the basket structure is made of steel, with panels of a borated aluminum to absorb neutrons.

Although during this thesis there have been work performed on the HI-STORM, the results and studies will not be shown due to a number of reasons, the main one being the proprietary nature of the cask and the information that was used. The second reason is that unlike most of the

results shown, in this case the results could not be validated against experimental results. Nonetheless this section is left to show the other type of cask that is available on the market.

Table 2-5. Fuel requirements for the HI-STORM (CSN, 2011)

Burnup max (GWd/MtU)	55
Enrichment range (in Uranium 235)	2.1 to 5%
Time in spent in the spent pool (years)	5 to 20
Maximum het load (kW)	0.9375

Figure 9. HI-STORM loading (CSN, 2011)

2.5.6 The Dry Cask Simulator (DCS)

The Dry Cask Simulator was an experimental cask manufacture by Sandia National Laboratories (SNL) to help validate CFD simulations under different thermal loads and internal pressures. This cask, unlike the previous ones is loaded with a prototypic BWR fuel assembly that is electrically heated (Durbin and Lindgren, 2017a; Lindgren and Durbin, 2017a; Pulido et al., 2019a). The cask has two configurations, the above ground, trying to replicate the behavior of casks like the HI-STORM, meaning in a vertical position and with the concrete overpack; and below ground where the casks are placed in a vault.

The BWR fuel assembly used for the DCS tests is a 9x9 rod configuration, with 74 rods, 66 full length rods and 8 partial rods, and two water tubes. The assembly is placed inside a canister, that is placed inside a shell that is open at the top, and has air inlets in the lower part, in Figure 10 the above ground configuration is shown. The temperatures are measured through thermocouples placed throughout the whole cask, including in the air region. The heat output power tested ranged from 0.5 kW to 5 kW, and from 100 kPa to 800 kPa.

- The fuel assembly is made of different materials, zircalloy for the spacers, water tubes and the channel box, incoloy for the rods, and magnesium oxide to simulate the uranium oxide.

- The basket cell, the canister and outside shell are painted carbon steel, with the exterior shell insulated with kaowool.
- The air inlets have a honeycomb structure facilitate the measuring of the air flow.

Figure 10. Dry Cask Simulator (Lindgren and Durbin, 2017a)

3 Computer Fluid Dynamics

In this section, a brief introduction to Computer Fluid Dynamics (CFD) can be presented. It is not an in-depth look, but it includes an introduction of their use and some of the main techniques employed in the discretization, the turbulence modelling and some best practice guidelines.

CFD is a branch of fluid mechanics that employs different numerical techniques and data structures to solve fluid flows. CFD solves the Navier-Stokes equations numerically, with different approximations. The development of the different techniques in CFD could be traced to Richardson (1922) (Hunt, 1998a) whose calculations on weather prediction, although flawed, paved the way to modern CFD and numerical meteorology. It was not until the 1960's that the development of three dimensional methods took off in Los Alamos National Lab (Harlow, 2004). In the early stages the aerospace industry led the development of the techniques, in fact the first published paper that solved a three dimensional problem (Hess and Smith, 1967) was from Douglas Aircraft Company. From that point, the work continued with further developments carried by Brian Spalding in the Imperial College of London, where a new implicit formulation was introduced as a way of coupling the velocity to the pressure, the SIMPLE algorithm (Patankar, S.V and Spalding, D.B, 1971). It was not until the 1980s that commercial codes were available with the introduction of codes such as the PHOENICS by CHAM (1980), FLUENT by Create (1983), STAR-CD from works conducted on the Imperial College (1987) or CFX-4.

Although initially the aerospace industry was the first adopter, nowadays CFD are employed in almost every industry due to its flexibility, cost and relatively ease of use. In fact due to the advantages when calculating aerodynamics profiles, drag and lift in the aerospace industry allowed a significant reduction on flight testing and wind tunnel hours from 77 wings tested on 1970s, to a mere 5 during the 2000s (Johnson et al., 2005). Although wind tunnel testing was and still is necessary, reducing the number of tests means faster and cheaper developments and shorter times to market.

These advantages not only are present in the aerospace industry, but in almost every modern industry specially from the expanded capabilities of the current codes that allows the user to solve multi physics problems, from multiphase, to chemical reactions, heat transfer, solid-fluid interaction etc. For example, reducing the amount of CO₂ emissions in the cement industry (Mikulčić et al., 2012), different improvements in the food industry, from packaging to bacterial growth (Norton and Sun, 2006), or to the safety of the nuclear industry (Andreani et al., 2008), (Yoo et al., 2010a) to mention just a few.

These improvements also reach into academia, where it has allowed the study of different problems, from buoyancy flows (Kumar and Dewan, 2016), to heat transfer (Cheng and Müller, 1998), to supercritical fluids (Rosa et al., 2011), just to name a few fields of study. There are thousands of research papers that use or evolve CFD each year (roughly around 6000 each year as per the web of knowledge).

3.1 Conservation equations

When studying fluid behavior, the conservation equations can be expressed either using an Eulerian approach or a Lagrangian approach. In the Lagrangian approach the particle or volume is followed as it moves through space whereas in the Eulerian approach a given volume represents a portion of space where material can flow through. Both methods can be used, and each has its advantages when studying different physics. All the works conducted in this thesis use the Eulerian approach to solve the conservation equation.

When studying continuum studies, the fundamental laws that govern the mechanics of fluids are the conservation of mass, linear momentum, angular momentum and conservation of energy, which in the differential form have this formulation (Moukalled et al., 2016):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad \text{Equation 1 Continuity equation}$$

Where ρ is the density (mass per unit volume), and $\mathbf{v}$ is the continuum velocity

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}_b \quad \text{Equation 2 Conservation of linear momentum}$$

Where $\otimes$ denotes the outer product, $\mathbf{f}_b$ is the resultant of the body forces (per unit of volume acting on the continuum), and $\boldsymbol{\sigma}$ is the stress tensor. For a fluid, the stress tensor is usually written as a sum of normal stresses and shear stresses $\boldsymbol{\sigma} = -p\mathbf{I} + \mathbf{T}$, where p is the pressure, and $\mathbf{T}$ is the viscous stress tensor.

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T \quad \text{Equation 3 Conservation of angular momentum}$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho E \mathbf{v}) = \mathbf{f}_b \cdot \mathbf{v} + \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\sigma}) - \nabla \cdot \mathbf{q} + S_E \quad \text{Equation 4 Conservation of energy}$$

Where E is the total energy per unit mass, $\mathbf{q}$ is the heat flux, and S_E is an energy source per unit volume.

3.2 Turbulence

In this section a brief introduction to turbulence will be presented. Due to the complex nature of turbulence and wide range of fields of study that deal with turbulence and its effects, this section will briefly explain what turbulence is, and some of the more common ways to model it in a fluid flow.

A standard definition of a turbulence flow would be characterized by chaotic changes in flow velocity and pressure, it can be observed in many everyday phenomena such as fast flowing river, storm clouds or a boat wake.

Whereas laminar flow is stable, turbulent flows are unstable, chaotic, with rapid mixing involving three-dimensional vorticity fluctuations, with a broad range of time and length scales (from below a millimeter to galactic scales). One of the most accepted theories of turbulence is the concept of “energy cascade” as developed by Kolmogorov (Kolmogorov, 1991a, 1991b)(edited and translated version). In Kolmogorov’s theory, turbulence is composed of eddies of different size, with the energy of the different eddies being dependent on the size of the eddies. The larger eddies transfer their energy to smaller eddies by breaking up, this chain of larger eddies breaking up into smaller eddies continues until the smallest eddy possible, at which point, the molecular viscosity is very effective at dissipating the turbulent kinetic energy as heat.

Using the concept of energy cascade, a direct solution of the Navier-Stokes equation for turbulent flow is possible but requires a very fine mesh (below the Kolmogorov’s scale), and very small time step to resolve the entire temporal spectrum. This approach is called Direct Numerical

Simulation (DNS), and is used very sparingly due to its large computational cost. It is possible that advances in computer technology (quantum computing) might make this approach viable for industrial flows but until such time, DNS is beyond most industrial applications.

To reduce the computational time and to simplify the resolution of turbulent flows, statistical analyses can be used. Statistical averaging techniques can be applied due to the time-dependent nature and wide range of time scales of turbulence. Unfortunately, time averaging leads to correlations that are unknown. These correlations constitute the classic closure problem of turbulent modeling. One such method is the large eddy simulation (LES) in which large eddies are directly simulated whereas small eddies are modeled using sub-grid scale models.

Although LES has seen more industrial and research use in the last few years due to advancing computing power the most common approach both in the industry and in academia (and the ones used in this thesis) is solving the Reynolds Average Navier-Stokes (RANS) equations. In RANS the approach is to decompose the flow variables into time-mean value component and a fluctuating one Figure 11, this decomposition is applied to all governing equations (Moukalled et al., 2016; Rieutord, 2015).

Figure 11. Fluctuating and mean variable components

Unfortunately, the set of RANS equations is not a closed set, and to solve it additional equations for the unknown Reynolds stress components are required. Calculating these stresses is what is called turbulence modeling.

Several turbulence models based on the Boussinesq hypothesis (Boussinesq J, 1877); in which the Reynolds stress are assumed to be a linear function of the mean velocity gradients. The models hope to express the turbulent viscosity, μ_t , in terms of a velocity $\sqrt{k}$, where k is the turbulent kinetic energy and length scales (ℓ) such that:

$$\mu_t = \rho \ell \sqrt{k} \text{ Equation 5}$$

These models are grouped into four main categories:

- Zero-Equation models, where an algebraic equation is used to compute μ_t , (Prandtl, L, 1949).
- One-Equation Models, where a single transport differential equation is used to compute the turbulent eddy viscosity (Baldwin and Barth, 1991).
- Two-Equation Models, where two transport equations are needed to calculate μ_t . This approach is the most widely used both in the industry and academia, due to its accurate predictions and relatively low computing time. More on these models in the next section.
- The second-order closure models (Daly and Harlow, 1970), which requires solving 6 equations (one for each turbulent flux) and therefore is the most expensive computationally.

3.3 Turbulence models

In this section some of the different turbulence models will be briefly presented, the focus will be those turbulence models that will be use throughout this thesis.

1.1.1 Standard k- ϵ model

One of the most used models is the standard k- ϵ developed by (Jones and Launder, 1972). It is a semi-empirical model based on model transport for the turbulent kinetic energy k , and its dissipation rate ϵ . One of the assumptions in the derivation of the equations is that the flow is fully turbulent and the effects of molecular viscosity are supposed to be negligible. Therefore, the standard k- ϵ model is a high Reynolds number turbulence model valid only for a fully turbulent flow, this model cannot be integrated all the way to the wall, within the boundary layer zone. In the model the turbulent kinetic energy k and the turbulent energy dissipation ϵ are calculated as:

$$\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho \mathbf{v}k) = \nabla \cdot (\mu_{\text{eff},k} \nabla k) + P_k - \rho \epsilon \quad \text{Equation 6}$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \nabla \cdot (\rho \mathbf{v} \epsilon) = \nabla \cdot (\mu_{\text{eff},\epsilon} \nabla \epsilon) + C_{\epsilon 1} \frac{\epsilon}{k} - P_k - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} \quad \text{Equation 7}$$

Where:

$$\mu_{\text{eff},k} = \mu + \frac{\mu_t}{\sigma_k} \quad \text{Equation 8}$$

$$\mu_{\text{eff},\epsilon} = \mu + \frac{\mu_t}{\sigma_\epsilon} \quad \text{Equation 9}$$

μ_t is the turbulent viscosity, k_t the thermal diffusivity.

When modeling part of a wall the standard k- ϵ introduces damping functions to some of the coefficients (C_μ , C_ϵ and $C_{\epsilon 2}$) in the model, this approach is usually called the Low Reynolds Number approach. The damping functions modulate the coefficients as a value of the Reynolds number incorporating the wall distance. In particular, the two Low Reynolds Number approaches that have been used in this thesis are:

- Standard k- ϵ Low-Re model (Lien et al., 1996a), the model uses the same coefficients as the standard k- ϵ model but provides damping functions that allow it to work in the viscous affected regions near walls, and it is recommended for natural convection problems (SIEMENS, 2018a)

- The AKN k- ϵ Low-Reynolds model (Nagano et al., 1994a), has different coefficients than the standard model and damping functions than the Low Reynolds variant. It is recommended for complex flows where the Reynolds number is low, such as compact heat exchangers (SIEMENS, 2018a)

3.3.1 Two-layer approach

The two-layer approach (Rodi, 1991), is an alternative to the low Reynolds number approach previously discussed. In this approach the flow region is divided into two layers. The first is the layer next to the wall where the dissipation rate ϵ and the turbulent viscosity μ_t are specified as functions of wall distance, far from the wall the values are calculated from the transport equations. The second is the layer above the first one and outside the closest zone to the wall. This process is no less empirical than the damping functions and the results are often as good or better than the damping functions approach (SIEMENS, 2018a).

Although strictly speaking the Realizable k- ϵ (Wolfstein, 1969a; Xu et al., 1998a), is not a two-layer approach, the variants used in this thesis have the two-layer approach, as they are a modified version of the Realizable k- ϵ . These models use a new transport equation for the turbulent dissipation rate ϵ , and the coefficient C_μ is expressed as a function of mean flow and turbulence properties, rather than being constant like in the standard formulation. These models are substantially better than the Standard k- ϵ for many applications and coupling it with a two-layer approach allows it to work with low Reynolds type meshes ($y^+ \sim 1$ or wall function type meshes $y^+ > 30$).

The $\overline{v^2} - f$ (Durbin, 1991a; Lien et al., 1996a) model solves two additional transport equations (besides k and ϵ), these equations are the wall-normal stress component and the elliptic relaxation parameter f , this is to determine the turbulent eddy viscosity. It can capture near-wall turbulence, which is critical for the accurate prediction of heat transfer (vital for this thesis), skin friction and flow separation.

3.4 Convection and turbulence modelling

Turbulence plays a critical role in heat transfer mechanisms due to its mixing capabilities, but in natural convection problems the transition between laminar flow and turbulent flow is complex. The more turbulent a flow is, the greater the Rayleigh number has (broadly speaking the Rayleigh number is the ratio between the time scale for thermal transport via diffusion and the time scale for thermal transport via convection at speed v):

$$Ra = GrPr = \frac{g\beta(T_s - T_\infty)L^3}{\nu\alpha} \quad \text{Equation 10}$$

Unfortunately, both the transition value, and its relationship with the Nusselt number is dependent on geometry, temperature difference, pressure, and fluid properties. Meaning that, both the transition point and the relationship between Rayleigh and Nusselt, are usually extracted from experimental results. For example the correlation for vertical surfaces as per (McAdams, William H., 1954a):

$$Nu = \left\{ 0.825 + \frac{0.387 Ra^{\frac{1}{4}}}{\left[1 + \left(\frac{0.492}{Pr} \right)^{\frac{9}{16}} \right]^{\frac{8}{27}}} \right\}^2 \quad \text{Equation 11}$$

Not only is the transition point difficult to actually know before hand, especially in complex geometries, but the nature of turbulent modelling means that one model does not fit all cases. Many studies have been conducted evaluating different turbulent models against different cases, in (Zhang et al., 2011), eight turbulent models were tested against four enclosed experiments from the literature, the four experiments included a natural convection case, a forced convection case, a mixed convection case and a strong buoyancy case, Figure 12. The eight turbulent models were the following: the zero-equation (0-eq) (Xu et al., 1998a), the RNG k-ε model, a low Reynolds number k-ε (LRN-LS) (Jones and Launder, 1972), the SST k-ω model (SST), a modified v2f model (v2f-dav), a Reynolds stress model (RSM-IP), the large eddy simulation (LES), and the detached eddy simulation (DES-SA). The models were evaluated for accuracy, with a qualification of A if the measured error is less than 10%, D for larger than 50%, with B and C with an error in between. The error for the mean temperatures is measured differently for each case, for example in the natural convection case the nominal temperature difference is taken as the difference between the hot and cold wall. In the next table the qualifications for each case is presented:

Cases	Compared items	Turbulence models							
		0-eq.	RNG k-ε	SST k-ω	LRN -LS	V2f-dav	RSM-IP	DES	LES
Natural convection	Mean Temp.	B	A	A	C	A	A	C	A
	Mean Velo.	D	B	A	B	A	B	D	B
	Turbulence	n/a	C	C	C	A	C	C	A
Forced convection	Mean Velo.	C	A	C	A	A	B	C	A
	Turbulence	n/a	B	C	B	B	B	C	B
Mixed convection	Mean Temp.	A	A	A	A	A	B	B	A
	Mean Velo.	A	B	B	B	A	A	B	B
	Turbulence	n/a	A	D	B	A	A	B	B
Strong buoyancy flow	Mean Temp.	A	A	A	A	A	n/c	n/a	B
	Mean Velo.	B	A	A	A	A	n/c	n/a	A
	Turbulence	n/a	C	A	B	B	n/c	n/a	B
Computing time (unit)		1	2 - 4		4 - 8		10 - 20	10 ² - 10 ³	

A = good, B = acceptable, C = marginal, D = poor, n/a = not applicable, n/c = not converged.

Figure 12. Qualifications for the different models (Zhang et al., 2011)

The results among RANS models (the ones that are viable for most simulations), show that the v2f-dav and RNG k-ε have the best performance overall, with the SST k-ω having problems for low turbulent flows.

3.5 Porous media

Porous media is used when it is needed to simulate a solid material that has a partially blocked area or number of pores or holes, for example honeycomb structures, packed bed chemical reactors or even nuclear fuel assemblies. Although it is a common tool in most CFD codes, each

code is different in how certain physics are implemented and coded, for simplicity and due to the fact that most of this thesis is done with STAR-CCM+, the porous media model will be explained as it is implemented in STAR-CCM+.

STAR-CCM+ has two ways in which the porous media can be implemented: the porous region, and the porous media model (as named in the code manual (SIEMENS, 2018a)). The porous region should be used when working with the physical velocity of the porous fluid is not a requirement and the solid and fluid phases are in thermal equilibrium. The porous media model on the other hand should be used when there are multiple solid phases. Physical velocity inside a porous medium is required when there is heat transfer between the solid and the fluid phases inside the region and other cases (for example for transient heat transfer analyses).

The porous media model has two ways to model heat transfer in the region: a thermal non-equilibrium model, in which the energy equation for the solid and the fluid is separated and have differentiated temperature. Unfortunately, this model does not allow the use of radiation (this means cannot be used for dry cask simulation). The second model is the thermal equilibrium, in which both the solid and the fluid energy are solved as one, meaning they share the same temperature, this model does allow thermal radiation.

As was stated before the pressure drop through these regions is done by modifying both the continuity and momentum equation as shown in Equation 11 and 12. The four variables needed are the porosity which is the ratio between the volume of the fluid and the volume of the solid, the tortuosity, that is the ratio between the length a particle must do to cross a porous media and the direct path, and the porous viscous and inertial resistance tensors, which modify the pressure drop as the velocity changes.

The equations for the thermal equilibrium can be found on

Continuity Equation:

$$\frac{\partial(\chi\rho)}{\partial t} + \nabla \cdot (\chi\rho\mathbf{v}) = 0 \text{ Equation 12}$$

Where:

- χ is the porosity
- $\mathbf{v}$ is the physical velocity
- ρ is the density

Momentum Equation

$$\frac{\partial(\chi\rho\mathbf{v})}{\partial t} + \nabla \cdot (\chi\rho\mathbf{v}\mathbf{v}) = -\chi\nabla p + \nabla \cdot (\chi\mathbf{T}) - \chi\mathbf{P}_v\mathbf{v} - \chi\mathbf{P}_i|\mathbf{v}|\mathbf{v} \text{ Equation 13}$$

Where:

- $\mathbf{P}_i$ is the inertial resistance tensor
- $\mathbf{P}_v$ is the viscous resistance tensor

Thermal Equilibrium Energy Equations

$$\frac{\partial(\rho E)_{eff}}{\partial t} + \nabla \cdot (\chi\rho_{fluid}H_{fluid}\mathbf{v}) = \nabla \cdot (k_{eff}\nabla T_{fluid}) + \nabla \cdot (\chi\mathbf{T}_{fluid} \cdot \mathbf{v}) \text{ Equation 14}$$

$$(\rho E)_{eff} = \chi\rho_{fluid}E_{fluid} + (1 - \chi)\rho_{solid}C_{p,solid}T_{fluid} \text{ Equation 15}$$

$$k_{eff} = \chi k_{fluid} + (1 - \chi) k_{solid} \text{ Equation 16}$$

Where:

- E is the energy
- H is the enthalpy
- K is the thermal conductivity
- C_p is the heat capacity

4 Dry cask modeling state of the art

As explained in section 2.5, with the increase need of dry cask systems and their ever expanding role, the need to understand the behavior of nuclear spent fuel during its phase inside a dry cask has also increased. In several meetings of the international community several gaps in knowledge were identified (Hanson et al., 2012; Sorenson and Kessler, 2012), after experts from Germany, Hungary, Japan, Korea, Spain, UK and USA, each supply a list of what they thought where the gaps in knowledge regarding dry cask systems. The consensus showed that the following gaps still remain:

1. Cladding:
 - a. Hydride effects
2. Canisters
 - a. General corrosion
 - b. Stress corrosion cracking
3. Cross-cutting gaps
 - a. Monitoring
 - b. Temperature profiles

Of these gaps this thesis will be mainly concern with the temperature profiles of the canister and the hydride effects since they are linked together through the Peak Cladding Temperature (PCT). The thermal limit of 400 °C (as per (USNRC, 2003)) is the temperature at which the hoop stresses reach 90 MPa, at this stress the hydrides dissolved in the clad can start changing orientation from an axial direction, to a radial direction. This reduces the critical stress intensity required to propagate a radial crack (Kim et al., 2010)(Kim et al., 2015; Singh et al., 2002)(among others). Other thermal effects include high temperatures on the concrete pad which may also degrade it due to dehydration (Alonso and Fernandez, 2004).

PCT can be calculated in a number of ways, through strict analysis of the thermal equations (although usually it is done by simplifying the model to 2-D) (Montefuel, 1993; Montefuel and Neil, 1993), or through numerical simulations with CFD codes such as STAR-CCM+ (SIEMENS, 2018a), ANSYS CFX (ANSYS, 2018), ANSYS Fluent (Baker, 2019) or Open Foam (Moukalled et al., 2016). Other codes use a Finite Element Method (FEM) to obtain the thermal behavior, like COBRA SFS (Pacific Northwest Laboratory, 2018a). Out of these options CFDs it is the most popular one, due to its flexibility (unlike codes such as COBRA SFS that can only calculate steady states in dry cask, CFD codes can be used for many different types of calculation), and large body of work (more on this in the following pages). Due to its increasing use for dry cask licensing in the USA, the NRC published a best practice guidelines document in 2013 (Zigh and Solis, 2013). The document gives guidelines in which uncertainties and user errors can be minimized.

Even though the best practice guidelines offer advice regarding the problem of simulating a dry cask system with CFD, it cannot provide validation of the results, to validate the codes and methodologies, experimental results are needed. Most of the experiments are conducted with dummy fuel assemblies with electrical resistances to provide the heat load, very few experiments are conducted using actual nuclear spent fuel (for obvious reasons). Besides the safety reasons behind the use of dummy fuel, there are other advantages such as being able to change the heat output or testing accident conditions during the experimental campaign (Lindgren and Durbin, 2017b).

One of the few experiments conducted with real spent fuel were the ones conducted on 1987 by EPRI using the TN-24P (EPRI, 1987a). These experiments have an advantage for testing different methodologies among them the results are public, there is enough public information regarding the geometry and materials so that it is possible to make a model of the cask; thanks to this the TN-24P is probably one of the most studied dry cask in the industry.

This cask has been used to validate specific codes such as COBRA SFS (EPRI, 1987a; Pacific Northwest Laboratory, 2018a). COBRA SFS is a code that performs thermal-parameter, finite-difference approach to calculate flow and temperature for spent-fuel storage and transportation systems. This code is derived from the COBRA family of codes and can be used both for steady state solutions and unsteady solutions (although the later are not recommended by the creators of the code). Although COBRA SFS presents an advantage in computational time over a CFD analysis, the pre-process of the code is complex and can be prone to user error. This is because the problem description, from the geometry to the boundary conditions, is introduced as parameters (rows and columns of numbers) Figure 13. These difficulties can be alleviated through the use of other external codes, for example writing the input based on Excel tables and Python scripts (Benavides et al., 2018; Galbán et al., 2018), errors found in the flow pattern in the solution, cannot be alleviated. A more in-depth description of these error and COBRA SFS will be presented in section COBRA SFS.

15	chan	44	36		
16		159.5	0.00		
17	1	1	256	0	0
18	1	1	0	0	1
19	1.13261.150.3314	2.19840.486	17.19840.486		
20	2.16061.226.6629	3.19840.563	180.1410.486		
21	3.16061.226.6629	4.19840.563	190.1410.486		
22	4.16061.226.6629	5.19840.563	200.1410.486		
23	5.16061.226.6629	6.19840.563	210.1410.486		
24	6.16061.226.6629	7.19840.563	220.1410.486		
25	7.16061.226.6629	8.19840.563	230.1410.486		
26	8.16061.226.6629	9.19840.563	240.1410.486		
27	9.16061.226.6629	10.19840.563	250.1410.486		
28	10.16061.226.6629	11.19840.563	260.1410.486		
29	11.16061.226.6629	12.19840.563	270.1410.486		
30	12.16061.226.6629	13.19840.563	280.1410.486		
31	13.16061.226.6629	14.19840.563	290.1410.486		
32	14.16061.226.6629	15.19840.563	300.1410.486		
33	15.16061.226.6629	16.19840.486	310.1410.486		
34	16.13261.150.3314	32.19840.486			

Figure 13. Channel description COBRA SFS

Other groups have use the TN-24P as a way to validate their CFD models and methodologies, in (Yoo et al., 2010a) 1/8 of the inside of the cask is modelled. The model has explicit representation of the fuel assemblies (meaning that the fuel rods are simulated), but the exterior boundary conditions are a fixed temperature in the inner wall of the canister. The study showed that a complete cask with temperature profiles for each rod can be modeled with accuracy. Once the model has been validated it can be used for further work, for example using the model to try to obtain a smaller scale model and then validate that against a dummy model (Yoo et al., 2010b). In (Yoo et al., 2019), the author tries to improve the thermal behavior of the cask by mixing the helium with high density inert gases (such as Xenon, CO₂, Krypton or Argon) at different pressures and mixing ratios. The idea was that by increasing the density of the gases, the increase buoyancy of the mixed gas would improve the thermal response. What was found

was that at lower pressures (up to 2.5 atmospheres), convection plays a negligible role, with conduction and radiation serving as the only relevant thermal mechanisms. At higher pressures some of the mixed gases showed small improvements to the thermal response.

(Brewster et al., 2012a) used porous media to simulate the fuel bundles in a model of half of the TN-24P. Once the results obtained were in line with the experimental results, one of the fuel bundles were changed to a fully detailed model of a fuel assembly (the fully modeled assembly consisted of 25 million cells). This last model showed very little difference with the porous media model. This study shows the two ways in which one might model fuel assemblies, the explicit model that represents the fuel assembly in detail (in this case extreme detail), with fuel rods, spacers, and the implicit way in which porous media is used to homogenize the fuel assembly into a single volume. These two philosophies regarding fuel bundle modelling have proved to be accurate with both cases having advantages and disadvantages. The explicit model has higher computational cost but on the other hand it does not require extra calculations such as equivalent thermal conductivity, pressure drop etc. (in Porous media, all these parameters will be determined *a priori*). The porous media model on the other hand is computationally less expensive, but it also is less flexible than the explicit model, if the problem to solve includes multi species, multi-phase physics or transient behavior the porous media might not be able to solve accurately these problems (some of the coefficients outline before are highly dependent on the fluid its properties and how they interact with the geometry making difficult their calculation). This discussion will be further expanded in 3.5.

Another example of using the different types of fuel representation can be found on the Modeling Validation Using the Dry Cask Simulator report (Pulido et al., 2019a) written by Sandia National Laboratories for the US Department of Energy it shows the results from five different institutions trying to replicate the thermal results of the dry cask simulator (Durbin and Lindgren, 2017b) (more of this experiment in The Dry Cask Simulator (DCS)). Each institution used a different set of codes, approximations, and boundary conditions. The five institutions are the Nuclear Regulatory Commission (NRC), Pacific Northwest National Laboratories (PNNL), Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT) and ENUSA S.A., S.M.E (Empresa Nacional del Uranio, S.A) in collaboration with the Universidad Politécnica de Madrid (UPM).

Table 4-1. Summary of modeling (Pulido et al., 2019a)

MODELING CONTRIBUTOR	CODE	FUEL REPRESENTATION
NRC	Fluent (CFD)	Porous Media
PNNL	STAR-CCM+(CFD)	Explicit
PNNL	STAR-CCM+(CFD)	Porous Media
PNNL	COBRA SFS (Subchannel)	Quasi 3D rods
CIEMAT	Fluent (CFD)	Porous Media
ENUSA-UPM	STAR-CCM+(CFD)	Explicit

The report concluded that porous media fuel representation can achieve modeling calculation results of peak cladding temperatures, average fuel temperatures, transverse temperatures and air mass flow rates that are comparable to explicit fuel representation. Other key observations were the following (Pulido et al., 2019a):

1. “Numerical uncertainty analyses: Future modeling efforts should include a rigorous estimation of modeling uncertainty to enhance interpretation of the results.

2. *Sensitivity analyses: Input parameters and choice of closure models should be explored and documented to gain a greater insight into model performance. These observations should be used to influence best practice guidelines.*
3. *Baseline numerical case: A single, baseline case with prescribed grid sizes and closure models should be performed by each modeling team to provide a more direct comparison of the underlying modeling physics. It is recognized that this recommendation is more applicable to CFD submissions and is likely not possible for lumped-parameter or subchannel models."*

Using the porous media model (Herranz et al., 2015) modeled the HI-STORM (2.5.5). In the study, several sensitivity analyses were performed, including local climate (external temperatures) and regionalization. The study found that the environment temperatures did not affect much the PCT, whereas heat load distribution or regionalization did have an impact on PCT (up to 21K increase). In (Lee et al., 2009) the porous media model was compared to a test case for both normal conditions, and off normal conditions (where some of the air inlets were blocked), in both cases the model could capture the main experimental variables.

If CFD tools could only be used to perform validation of existing experimental results, they would not be very useful (whether in the nuclear industry or others). In this sense other works have proposed new ways in which a dry cask could be improved, as previously explain this could be using a gas mixture (Yoo et al., 2019), or introducing heat pipes in the fuel elements of a dry cask to lower its temperature (Jeong and Bang, 2016). This study showed that heat pipes (are passive heat transfer devices that use both conduction and phase change to extract heat from a source), are capable of lowering up to 95 K the PCT when five heat pipes were used for each assembly. The authors proposed coupling such assemblies to Stirling motors to improve even further the efficiency of the system. Although heat pipes on dry cask was shown to be useful for lowering the temperatures inside the cask, maximum temperatures are not the only safety limit to consider, mechanical limits could prove to be a challenge if such mechanisms were to be implemented. Other studies provide more conservative changes that could be relatively easily to implement like adding undulations or semi-circular fins that can increase the heat transfer coefficient in a concrete type canister (like the HI-STORM) three orders of magnitude (Remache et al., 2019).

5 Methodology

In this chapter, the methodology of the thesis is presented, along with the reasons behind the need for such methodology. The steps taken to develop it will be explained from the first steps in creating the model (geometry creation, meshing, etc.) to the final steps that were taken to ensure that the results have the desired quality and certainty.

5.1 Objectives and phases

The main objective of this work is to develop a methodology that can accurately calculate temperatures distribution inside and outside a dry cask system with reasonable computational effort, without the necessity of a high-performance calculation server. This is a very important goal, as not all organizations that work in dry cask simulation have HPC resources.

The steps of the core methodology (i.e., the thermal calculation of the cask) will be presented as an evolution, firstly how these works started and how different aspects of the methodology have evolved to ensure the quality of the results thanks to the effort put into the validation of the methodology. Once the core methodology has been explained, the extended methodology will show how this work can be used to tackle other problems concerning casks, based on a solid foundation. Finally, the two experiments that have been used to validate the methodology will be shown, and some of the limitations regarding the models developed.

The core of the methodology consists of several iterative steps. First, the methodology begins with the planning stage in which the cask is simplified. Then, the process continues in the pre-process phase, which includes boundary condition selection, selecting physics and numerical schemes, meshing, etc. Unfortunately, each CFD code does things differently, both in terms of naming convention and algorithm, to prevent this work from turning into a user's guide to "How to make cask in code X", some of the explanations will be general, with examples from STAR-CCM+, Fluent or CFX.

5.2 Model creation and best practices

In this section, some of the key steps in creating a cask model with a CFD code will be shown, most of the steps in this section are done before the model is run. This section should be taken as a guide and in certain sense as a best practices guideline. Some of the tools and operations explained here are specific for STAR-CCM+ code since that is the code that has been used more frequently in this thesis, nonetheless most CFD codes have similar tools (the name is usually different, for example "Directed Mesh" in STAR-CCM+ is called "Sweep" in Ansys Meshing).

5.2.1 Geometry

Although the process of geometry creation and meshing can be thought as independent and done in sequence they are extremely intertwined and it is important to take into consideration when creating the geometry how it affects the meshing process.

The first step in the model creation process is creating a CAD model of the cask. Depending on the available information, this process might vary. If the detailed engineering drawings are available, the process should include a simplification step, which means that the geometry should be modified in a way that facilitates the simulation without affecting too much the geometrical precision. Simplifications should be done to reduce the final mesh and body count; all simplifications must ensure that the final solution is not affected or that the impact is minimal. Some of the simplifications regarding a dry cask geometry can include:

- Eliminate structural components such as bolts, welded lines, nuts, etc. These components have limited thermal impact but would have large impact in the meshing process and would increase the computational requirements.
- Complex bodies such as the neutron shield ring can be modified from several bodies to a single body with the use of equivalent thermal conductivities. As an example, it can be seen in Figure 14 the modifications performed to a prototypical neutron shield (more on the thermal side on the next chapter). This modification will decrease the number of bodies and contacts, simplifying the mesh process and reducing errors such as lack of contact between bodies.
- Closing small gaps between two bodies, this may prevent the fluid from moving across the gap and should be taken into consideration whether this effect and how it is changing the solution. There are two reasons behind closing these gaps: the first being that meshing such gaps throughout the whole cask might make meshing the model an extremely difficult task and will significantly increase the computing time of the model (if not making it outright impossible to run in most computers). The second reason is that those gaps might close once the cask has reach a steady state condition due to thermal expansion, as will be further explored with a FE Mechanical analysis. These closed gaps can then be simulated using thermal resistances, limiting the thermal impact.
- Fuel assemblies and how to simplify them will be tackle in the chapter DCS, nonetheless simplifying the fuel assemblies is one of the core steps in building the cask model. Due to the extremely complex geometry of a fuel assembly, and the surrounding fluid, the fuel assemblies must be simplified to a degree, unless one has access to an extremely powerful computer and time is not a constraint. As a named example, in (Brewster et al., 2012b) a single assembly is fully modeled, but that single assembly and its surrounding fluid reach up to 25 million cells more than any of the simulations in this thesis. This decision will have to be an equilibrium between the detailed needed, the problems to be solve and the computer resources available.

Figure 14. Neutron shield change

The next step after deciding on the simplifications and constructing the CAD model is slicing the bodies up so that the meshing operations can be done as streamline and flexible as possible. Although the automatic meshing operations that most CFD provide have greatly improved in recent years, they are still lacking when tackling difficult geometries like the fluid surrounding

the fuel assemblies. In this case when automatic mesh is used the user has less flexibility when performing refining or coarsening operations, especially if the refining or coarsening has a preferential direction.

In Figure 15, the slicing sequence for the fluid region of the TN-24P is shown as an example, first the fluid surrounding the fuel assemblies is sliced at the top and the bottom of the fuel clads. Depending on the code, bodies like the inferior plenum (Figure 15 bottom right) might need further slicing to allow greater control over the mesh creation process and to allow for extruded or directed meshing. Slicing the bodies tries to make each body in the geometry sweepable or projectable; meaning one or various surfaces can be projected into the opposite surface or surfaces and if this projection fills its own volume completely then it is sweepable, more on this operation further down in the chapter.

Figure 15. Preparing the fluid region

Once the bodies have been sliced, one of the most crucial elements is ensuring the correct contact between bodies. In some codes there are automatic tools that do this operation with certain level of precision (in STAR-CCM+, in the CAD module the operation is called *imprint*). Nonetheless, it is highly recommended that both the contacts and the CAD quality are checked, this step - although tedious - might prevent future errors from surfacing. In some cases, the code will not detect geometry overlapping or lack of contacts between two adjacent surfaces and the simulation will diverge in only a few iterations (some of these errors are difficult to detect and troubleshoot). In some codes this mistake will be corrected in a relatively small amount of time, whereas in some other codes these errors can mean starting the setup almost from the meshing step and have a large impact on time. Some of these errors are due to lack of quality when importing the CAD into the CFD code (even when the CAD was created in the specific CFD environment). For example, in Figure 16 two errors are shown, in this case both the CAD and the CFD model are from the same environment (STAR-CCM+). In others it can be user error, or errors during the mesh creation process.

Figure 16. Errors during CAD import operation

A full cask has thousands of bodies and surfaces, for example the $\frac{1}{4}$ of the TN-24P has over 1350 bodies and more than 7000 surfaces. To keep everything manageable it is highly recommended to group bodies together usually by their material properties or their placements in the geometry (this is up to the user). For example, all the clads together or the different sliced region of helium by geometric familiarity (the helium surrounding the clads together in one group, upper and lower plenum in another, etc.). The end goal is to have a model in which finding certain body or surface is fast and streamlined. This will help during all the following steps, from meshing all the way to post processing.

After grouping the bodies, the next step is to name those surfaces that are of interest. At a minimum the boundary conditions need to be named, but it is recommended to name some other surfaces, especially those that might prove useful during the mesh or post process step. Some codes allow (Ansys) for selecting and naming surfaces and bodies based on any number of geometric criteria; when this is possible, it is a great tool to use. Other codes unfortunately do not allow this kind of selection (STAR-CCM+), therefore manual or macro work is recommended to accomplish these tasks. This organization and clarification process will help troubleshoot problems, speed up setting up the boundary conditions, and make post-processing faster.

5.2.2 Meshing

Meshing is one of the most crucial steps in CFD simulations. It will determine the quality, accuracy, convergence, and the computing time of the results (other factors include the selected boundary conditions and the physics selected for the model). As previously mentioned, every code has different algorithms for meshing, with specific tools and criteria, therefore the recommendations that follow are general, and although the naming conventions are different most codes have similar tools.

As stated before, the objective of slicing the geometry into blocks is to create bodies that are sweepable. A “Sweep Mesh” (Ansys) or “Directed Mesh” (STAR-CCM+) creates a 2-D mesh in one of the surfaces in Figure 17 that would be in X-Y plane, and then the mesh is projected along an axis, in this case Z axis. This type of mesh allows for great control over the mesh, especially in bodies like the fluid inside a fuel assembly, where the axial levels can be stretched in the same direction of the flow. Without this type of mesh, meshing a fuel assembly would require a large number of cells due to the small pitch between fuel clads (a few millimeters). As will be further explore with the Grid Convergence Index, the number of axial divisions has an impact on both quality and computing time, for a dry cask in steady storage mode (i.e. no accident condition or multi-phase flow). As a lesson learned from experience, the sweet point (the compromise) is between 60 and 80 axial divisions, below 40 leads to instabilities and divergence problems, and above 100 the accuracy does not increase, whereas the computing time does.

Although it is usually not recommended to stretch the mesh and skew the aspect ratio of the cells, in this particular case it will not impact the quality or convergence (further clarification in Grid Convergence Index) of the results because the stretching is along the main fluid direction (there is barely any cross flow between channels), and the velocities inside the channels are limited to a few millimeter per second. This method of meshing is highly recommended for all the bodies inside the cask. In some bodies it may not be possible and only an automatic meshing procedure is possible, the use of local or volumetric controls may achieve equivalent results. For bodies like the outside air of the canister automatic meshing is recommended since a boundary layer is required.

Figure 17. Sweep or directed mesh

Once the mesh is done, checking the quality of the mesh is recommended, in this case most codes have automatic and specific tools to measure different quality parameters of the mesh. In general, the user must check the following:

- Is the mesh dense enough in zones with high-gradients of the target variables?
- Is the distribution between high and low gradient areas optimal?
- Are there enough layers near the walls for turbulent and heat transfer effects?

On a local level the user should check each code specific quality indicators because each code has different ways in which they measure and report the quality parameters, nonetheless some of the most common are:

- Orthogonality: it is related to how close the angles between adjacent element faces are to some optimal angle (depends on the type of mesh).
- Skewness: it is the angle between the face area vector connecting two cells and the vector connecting the two cell centroids
- Aspect ratio: it is the ratio between length and height (in 2-D)
- Volume change: it is the ratio between the volume of a cell to that of its largest neighbor

Although these parameters are important when preparing the mesh, they are hardly ever reported in the literature, likely because each code calculates and reports the values differently. After the mesh has been constructed, some codes allow the user to see the interface mesh between bodies, for example, between a fluid region and a solid region), therefore it is easy and recommended to see if there are holes in the interface that will affect the end results Figure 18 shows a bad interface between the fluid and solid region.

Figure 18. Badly mesh interface

5.3 Core Methodology

In this section the steps of the core and extended methodology will be explained, together with the reasons behind choosing each model and how it has been validated against the experimental results. This section will also give a brief overview of the evolution of the models from the beginnings of the project to the final results, this is important since some of the advances and discoveries have taken place after the core methodology was developed, in those cases it will be reflected on the text.

The first part will introduce the beginning of the methodology, which began before this work was thought as a PhD, then the core methodology developed for this thesis will be presented, and finally and an introduction to the works that been born from this core methodology will be briefly explained. These other works represent expansions of the core methodology. These works have been named extended methodology due the links to the previous works and that they are based on the works of the core methodology. The results for each model and step will be explained in the Results section.

The core of the methodology is a two-step approach to modelling the nuclear dry cask, in the first step the cask is modelled from the interior wall of the canister to the surrounding area (air and concrete pad). From this exterior model the boundary conditions for the interior model are extracted, this exterior model also shows the thermal impact the cask has on the environment, and the environment on the cask. An schematic of the methodology is represented in Figure 19.

Figure 19. Methodology diagram

In the second step the interior of the cask is modelled from the inner surfaces of the fuel clads to the outer layer of the cask without the surrounding area. This model provides temperature distributions, PCT, thermohydraulic behavior inside the cask and heat fluxes. These heat fluxes and their distribution are then re-introduced into the exterior model, improving the precision of the model. This iterative process is carried out until convergence of both models is reached

(usually one or two iterations, since the change from one iteration to another is usually not great). This two-step coupling allows the model of the cask to obtained great precision without a huge computational load.

5.3.1 Preliminary works

The origins of the methodology started in a bachelor degree thesis called “Evaluación térmica de un contenedor de combustible nuclear gastado con dinámica de fluidos computacional” (Thermal evaluation of a spent nuclear cask using computer fluid dynamics) (Benavides, 2015). The work on that project started in September 2014 with the idea of modelling the DPT dry cask with a CFD code. Initially that code was going to be OpenFoam, but limited time and experience, proved to be too great a challenge, therefore the code that was used in the end was Ansys Fluent.

In order to obtained valuable information regarding the exterior of the cask, the boundary conditions for the interior model, measured the thermal impact of the cask on the environment, reduced the computational load and finally as a first learning step in CFD modeling, the study of the cask was split into two models one exterior model and one interior model; instead of an interior model with a calculated external boundary conditions as it was usually done. The exterior of the cask was modelled from the inner surface of the cask wall to a region of both air a concrete surrounding the cask. The interior model was done with fuel represented by the void left on the helium by the fuel clads to the outer walls of the cask. In Figure 20 the two models are represented.

Figure 20. DPT models, exterior model (left) and interior model (right) (Benavides, 2015)

These models were the foundation from which the actual methodology was born. Since then, many of the initial hypothesis have been proven wrong (for example, the way that the fuel was represented), nonetheless many of the initial studies proved successful. Among the successful studies conducted were symmetry studies for the outside of the cask, mesh independence studies (it would eventually evolve into the method outlined in Grid Convergence Index section) and radiation studies.

Probably the most challenging task performed in this preliminary work was meshing the interior cask, especially the helium surrounding the fuel assemblies. Many of the lessons outline in the section Geometry , were developed during this initial work. This initial work provided some insight into the inner workings of a nuclear dry cask, with results showing temperatures like in Figure 21, or the thermo-hydraulics like in Figure 22, and that it was possible to obtained results for a dry cask using CFD codes.

Figure 21. Temperatures inside the DPT (Benavides, 2015)

Figure 22. Streamlines of the upper plenum in the DPT (Benavides, 2015)

5.3.2 Fuel assemblies

Simulating the interior of the cask means choosing a way to simulate the fuel assemblies. There are several ways in which one might simulate a fuel assembly:

- The most complex one being simulating the fuel assembly as it is (fully detailed), this method has the advantage of not having to estimate or guess any properties in the fuel assembly and how interacts to the surrounding environment (both in terms of heat transfer and fluid dynamics). Unfortunately, as was previously mentioned, this method is computationally prohibitive (Brewster et al., 2012b).
- On the other side of the spectrum, is using porous media to simulate the fuel assemblies and the surrounding fluid. This method which turns the geometry into a homogeneous body with equivalent properties has the advantage of being computationally cheap, and the pre-process is significantly easier to tackle (it does not have a large number of bodies or surfaces), but unlike the explicit method every thermal and hydraulic property has to be pre-calculated or guessed, making use of this method less flexible and very dependent on the user experience.
- The third method is using an explicit fuel assembly in which the fuel assembly is represented at least by the clads, the rest of the components may or may not be included, simplified, or modified to meet the requirements of the problem. By using this approach to simulate the fuel assembly the number of pre calculations is reduced to a minimum (or outright disappears), and the computer resources are kept at a reasonable level (1/4 of the TN-24P can be meshed in 4M cells). The other components of the fuel assembly, and whether they have an impact on the accurate prediction on temperature will be discussed in DCS. In Figure 23, a sketch of a real fuel assembly (left), an explicit representation of a fuel assembly without other components, and a sketch of a porous media fuel assembly right is shown to explain the different approximations.

Figure 23. Real Fuel assembly (sketch) (US NRC, 2020a), an explicit fuel assembly and a porous media fuel assembly

In this work, the third method is used, as the fuel is represented by each individual clad. This way there is no need to approximate the properties or the interaction between the components, and without the huge computational load of a fully detailed fuel assembly.

Some lessons learned from the preliminary works section should be outlined:

- The fuel assemblies were initially modelled as the hole left on the surrounding helium, the heat flux imposed in that first layer of helium. This approximation meant the simulation did not have to consider the bodies of the assemblies, only the surrounding fluid, unfortunately it was not until the model of the TN-24P was simulated that the shortcomings of this method became evident.
- The main error was that by not including the clads there are no thermal resistance between the heat flux and the fluid, this means that the temperatures are significantly higher. Not only that, by erasing the fuel clads and pellets the axial heat transfer is eliminated (even if it is small to begin with), every watt has to go directly into the fluid. In Figure 24 a schematic 2 D representation of the thermal resistance system with and without clads, and a model of a single assembly without and with clads (top and bottom respectively). In all cases $T_{interface} > T'_{interface}$ and $T_{fluid} > T'_{fluid}$. This was initially saw in the full model of the TN-24P Figure 25, it was then tested in a single assembly and verified by using thermal resistances.
- This problem also appears when eliminating the fuel pellets and leaving just the clads, but unlike when no solids are present, the impact was significantly smaller with temperature differences of around 6 °C, this was seen as an acceptable error since it significantly reduces the computer times and requirements. This error can be further reduced by using equivalent thermal properties, unfortunately these changes were tested after most work on this thesis was conducted therefore, they will not be included in this work.

Figure 24. Schematic thermal resistance for a system without clads (top) and with clads (bottom), on the right a simulation of a single assembly with and without clads

Figure 25. With and without clads inside the TN-24P, versus experimental results

5.3.3 COBRA SFS

As was briefly mentioned in previous chapters, the COBRA SFS has been used to calculate temperature distributions inside a cask. Initially this code was going to be used as a complimentary code to STAR-CCM+, but an error found in the flow pattern during the initial phase of this thesis was found and it could not be solved in time.

The error consisted of the fact that the flow from the upper plenum to the lower plenum, instead of being distributed throughout all the channels in the periphery (as it should), it is directed to just two channels Figure 26. This error was reported to the code creators, whom confirmed that the error was happening when the upper plenum model was used. The results (thermally speaking) were fairly accurate, but this is mostly due to the fact that the TN-24P is a low pressure cask (1 atmosphere when it is loaded), therefore convection plays a relatively small role in dissipating the heat, the error would be compounded as the pressure (and therefore the convection), is increased (Yoo et al., 2019). This error was estimated severe enough to stop using the code for this thesis.

Figure 26. Helium Flow in the TN-24P (velocities in mm/s). Blue is downward direction and red upward

5.3.4 Interior and exterior model

In this section the methodology for the two-step approach, outlined previously, will be further expanded and justified. Unlike the preliminary methodology, this actualized methodology has been constructed and validated by using experimental results, which are outlined in section Experiments. Thanks to the data from the experiments some of the initial hypothesis have been found to be incorrect, these will be outlined. The reasoning behind splitting the simulations into an exterior and an interior model for simulating the thermal steady state of a dry cask are the following:

- Obtaining realistic boundary conditions that can be changed to the user specification without needing to guess the value for heat transfer coefficients or outside temperature. In the best practice guidelines written by the US NRC (Zigh and Solis, 2013), it is proposed the use of constant values obtained through the use of correlations for the heat transfer coefficient value. Although this allows for faster creation of the models, it lacks precision and flexibility. Precision because by using a correlation that is meant for vertical flat surfaces (Churchill and Chu, 1975) or horizontal surfaces (McAdams, William H., 1954b), means that the approximations cannot capture the complexity of a dry cask. And flexibility because these correlations cannot take into account weather effects like wind, solar radiation, rain, the presence of other casks or accidents like a fire or a flood. Whereas by using a simulation these effects can be simulated. As an illustrative example, on Figure 27 the temperatures and the heat

transfer coefficients (left and right respectively) on the neutron shield, calculated (Churchill and Chu's correlation and simulated on the exterior model).

Figure 27. Temperature (left) and heat transfer coefficient (right) on the neutron shield simulated versus calculated

- Reducing the computational load compared to a fully coupled simulation, where both the interior and exterior are modelled. In some cases, simulating the air is reasonable, due to the small volume of air to simulate, this is the case of casks like the DCS or the HI STORM.

The process of taking the boundary conditions from the exterior model was initially done by extracting the values from the surface in question, like in Figure 27, and fitting a polynomial curve to the values. The polynomial was then introduced into the interior model as a boundary condition. Although this way of is valid and most of the results from this thesis is performed in such a way, a more recent development allows for the direct coupling of both models. With this new approach the values extracted from the exterior model are interpolated directly into the mesh of the interior model.

When the boundary conditions of the interior model (heat flux to the exterior) are introduced to the exterior model, the new method instead of averaging the total heat flux per surface and using this constant value for the interior boundary condition (for example in the case of the TN-24P 92% of the total heat flux is through the lateral walls), uses the values extracted directly from the interior model. For example, Figure 28 shows the heat flux on the inner surface of the top lid; on the left the constant value (first method), and the mapped method on the right.

To accomplish this a Python script was developed that allows the values from the quarter cask to be converted into a whole cask (the initial values do not have to be of a quarter, as long as the angle of the symmetry is a multiplier of the circumference). The script assumes that values are symmetric and equal for the same height. The advantage of this development will be further shown in section TN-24P.

Figure 28. Heat flux constant and directly mapped to the inner surface of the top lid

5.3.5 Grid Convergence Index

To guarantee that the results are mesh independent, studying it is part of ensuring the quality of the results in a CFD model. There are many ways in which a mesh independence study can be tackled, from studying how the variable of interest changes as the mesh is refined, to extrapolating the results to an infinite fine mesh, (this is called the Richardson extrapolation (Hunt, 1998b)), or the Grid Convergence Index (GCI) as introduced by (Roache, 1994). All these methods are valid, for this work the GCI was chosen. The GCI is a way to standardized, measured, and quantify the uncertainty in simulations.

To perform the GCI, a simulation is run in several meshes with each mesh being refined, until the values for the GCI are considered acceptable. The grid refinement ratio (r) is defined as the ratio between the grid size of the different meshes, equation 17 shows that the value for a 3-D grid size (h) is.

$$h = \left[\frac{1}{N} \sum_{i=1}^N (\Delta V_i) \right]^{1/3} \text{ Equation 17}$$

The refinement ratio should be kept as constant as possible, this is extremely difficult in real world scenarios where the geometry is complex. For example, the interior cask model is made of a large number of bodies and regions, both solid and fluid. Since the refinement of the meshes could not be done globally the refinement was done to the most important regions for the variable of study (PCT) which are the fluid regions and the clads themselves.

To calculate the GCI, the first step is to calculate the observed order of convergence of the simulations, although normally the codes have an order of convergence that can be selected, the reality is that the actual order of convergence changes due to numerical errors, the mesh, etc. The observed order of convergence is calculated as follows:

$$p = \ln \left(\frac{f_3 - f_2}{f_2 - f_1} \right) / \ln(r) \text{ Equation 18}$$

Where f_i is the value of the variable of study, if the ratio r is not constant, then p is calculated in an iterative manner as:

$$p = \omega \rho + (1 - \omega) \frac{\ln(\beta)}{\ln(r_{12})} \text{ Equation 19}$$

Where ω is a relaxation factor (usually taken as 0.5 as per (Roache, 1994)), ρ is the value of p in the previous iteration, and β is defined as:

$$\beta = \frac{(r_{12}^\rho - 1) \varepsilon_{23}}{(r_{23}^\rho - 1) \varepsilon_{12}} \text{ Equation 20}$$

Where ε is the relative error between meshes:

$$\varepsilon = \frac{f_2 - f_1}{f_1} \text{ Equation 21}$$

Finally, the GCI between the fine mesh and the medium mesh is calculated as:

$$GCI_{12} = \frac{F_s |\varepsilon| r_{12}^p}{(r_{12}^p - 1)} \text{ Equation 22}$$

Where F_s is a safety parameter (usually with a value of 3, if just two meshes have been employed and 1.25 if 3 meshes have been used (Roache, 1994), and for the medium and coarse mesh the value is

$$GCI_{23} = r^p GCI_{12} \text{ Equation 23}$$

This method although it seems cumbersome, especially compared to other simpler methods, ensures that the numerical uncertainty is quantified and reported in a consistent manner, and in particular in order to speed the calculations, a Python script was developed that made the whole process fast and reliable.

5.3.6 Turbulence modelling

Turbulence modeling and its impact on natural convection and heat transfer is a complex matter as has been outlined in the Dry cask modeling state of the art. When checking whether a fluid flow is turbulent or not, the Reynolds number is used in forced convection cases and Rayleigh number in natural convection (Incropera et al., 2013). The Rayleigh number is the product of the Grashof number (describes the relationship between buoyancy and viscosity) and the Prandtl number (ratio between momentum diffusivity and thermal diffusivity), the transition between turbulent and laminar flow is usually 10^9 .

$$Nu = \frac{hL}{k} \text{ Equation 24}$$

$$Pr = \frac{\mu C_p}{k} \text{ Equation 25}$$

$$Gr = \frac{L^3 \rho^2 g \Delta T \beta}{\mu^2} \text{ Equation 26}$$

$$Ra = Gr Pr \text{ Equation 27}$$

In this methodology, two different situations are presented:

- The exterior models present turbulent characteristics with values exceeding the laminar values. In these simulations the use of a turbulent model is necessary. As it will be shown in the Results, most of the turbulence models tested are accurate enough to predict

temperature distributions on the outside of the cask, but there was no significant difference between the different models to assess which one is better for these simulations. Therefore, it is the user's experience and with help from the user's manual for each code that the user has to choose.

- The interior model is significantly more complex: the inner pressure drives the change from conductivity-based heat transfer to convection based, and with it the increase in turbulent flow. The lower pressure cases (around 1 bar) have Rayleigh numbers below the transition point, whereas the higher pressure cases are in the transition zone (around 10^9), in these simulations a study between turbulent models and laminar models show be done. In the lowered pressure cases, although the Rayleigh number is below the transition point, this author recommends doing a turbulent study to see whether it has an impact on the temperature distribution and convergence criteria. In codes such as STAR-CCM+, the change in temperature distribution and values is negligible whereas the impact on convergence is not since it seems the code reaches convergence faster and better with a turbulent model. In some other codes the impact in temperature distribution is large enough that the turbulent model overpredicts the convection significantly changing the temperature distribution.

5.4 Extended methodology

In this section the extended methodology will be briefly presented, with the reasons behind each study. The extended methodology contains those works that have been done based on the previous methodology, but with a different objective and answering different questions. Whereas the first part deals with the temperatures inside and outside of a single cask, these extended works include several casks in temporal storage, the mechanical performance of the cask under the thermal load of the assemblies or the drainage process of the cask. These later studies are just some of the applications which this methodology could be applied to.

5.4.1 Drainage process

Before the casks are taken into the storage facility the cask has to be loaded, drained and has to be dry, in a process that was explained in Dry cask systems. These complex steps are a challenge to simulate, besides running a transient simulation, multiple species (helium and water) and phases (liquid and gas) interact with one another.

The methodology gave initial steps towards simulating these complicated physics, simulating part of the drainage problem and the drying step.

5.4.2 Temporal storage

Most thermal calculations of a dry cask are performed with a single cask in mind, but the reality is that casks are storage together they can be placed in an outside facility or inside facility. In both cases the cask being near one another means, that radiation is lowered, even if one cask is cooler than the others it is still hotter than the environment. Convection can be also impacted since in the surrounding air must cool more heat output, in Figure 29 an interior and exterior facility are shown. In Figure 29 it is clear that the casks are very placed together very closely, impacting the thermal performance.

Figure 29. Interior storage facility (left (ENSA, 2014) and exterior facility (right (US NRC, 2020b))

With the use of the methodology, results both for the outside and inside of the cask can be made, both to measure the impact, and whether it could surpass the safety limits; and eventually facilitate thermal positioning inside a storage facility when spacing is limited.

5.4.3 Mechanical Calculation

As will be shown in TN-24P one of the variables that have the largest impact on the PCT are the size of gaps between canister and basket. These gaps not only impact the maximum temperature of the cask but also on the thermohydraulic of the whole cask. When this first gaps were tested on the beginning of this thesis they could only be modeled as thermal resistance as simulating them would require prohibitive computer resources, and due to the uncertainty of the size of the gaps they could only be modelled as constant.

By using the results of the interior cask, the temperatures can be extracted, and introduced into a mechanical analysis code such as ABAQUS (ABAQUS, 2017). ABAQUS is Finite Elements code (FE) that allows the user to analyze mechanical behavior, in order to accomplish this coupling a new methodology had to be developed. This methodology was developed with the collaboration of the research center Jožef Stefan Institute of Slovenia. Although both codes allowed for co-simulation (meaning that the simulation is run simultaneously on both codes, every few iterations the codes refresh the input from one another), this could not be done due to licensing limitations of the codes.

When co-simulation is not necessary both STAR-CCM+ and ABAQUS offer the possibility to run sequential simulations using a third external file, the process is explained by STAR-CCM's user manual using the algorithm on Figure 30 (left). In this method the model would be prepared in ABAQUS, imported into STAR-CCM+, then the model would be run and exported, by mapping the results into the meshed prepared in ABAQUS. This method is cumbersome and means that if the mesh in ABAQUS has to be changed, the process has to be started from the beginning.

Since STAR-CCM+ allows the results to be exported directly into a neutral file as mapped values (the value of each cell and its position), this file was then introduced into ABAQUS using a mapped field to be used as a volumetric (or surface) boundary condition, then ABAQUS interpolates (or extrapolates) the results into its own mesh, eliminating the need to go back into STAR-CCM+ when a new mesh is required.

This work allowed us to see what happens to the gaps in the cask when thermal load is applied and reduces the uncertainty of the gaps.

Figure 30. Algorithm for coupling simulations, left as explained in the User's Manual of STAR-CCM+ (SIEMENS, 2018a) and right the developed methodology

5.5 Experiments

In this section the two experiments that have been used to test the methodology are presented, in both cases the results and the components are accessible and public (these are the reasons why these experiments have been chosen). Even though the information is public, not everything that is required is available. In the case of the TN-24P, although the materials and general description of the geometry is available, but it is not complete, for example there are no engineering drawings, and some of the materials are not specified. In the latter section of each experiment a discussion on the limitations of each of the experiments will be provided alongside the expected impact on the end results.

5.5.1 TN-24P

The experiment was conducted at the Idaho National Engineering Laboratory (INEL). The objective of these test was to establish one or more storage technologies that the NRC may approve for use at civilian reactor sites while also collecting the data necessary to assist utilities in the licensing activities. The TN-24P was one of the casks selected for testing, the design and manufacturing of the dry cask was conducted by Transnuclear Inc.

Dry cold runs with dummy fuel assembly were performed to test procedures and gain operating experience. The PWR fuel was tested to ensure integrity before the assemblies were taken from Surry Nuclear Power Plant to the experimental site.

The fuel assemblies consisted of 15x15 fuel rods with 21 guide tubes, top and bottom nozzle and seven grid assemblies, Figure 31. The code ORIGEN2 was used to predict decay heat in the fuel assemblies, using data from the life cycle of the fuel assemblies) reactor operating histories, decay times after final cycle of operation, monthly measured fuel assembly relative power density, etc.). The predicted decay heat for the 24 assemblies was 20.6 kW at the start of the experiment and 20.3 kW at the end of the experiments. On average each assembly had 850 W, with the individual ranging from 830 to 919 W, the initial enrichment ranged from 3.2% to 2.91%, and the burnrup (GWd/MTU), was 31.5 for the highest and 29.8 for the lowest. The axial decay heat profiles were developed using axial gamma radiation scans, see Figure 32. The fuel assemblies were loaded to have the most symmetric load pattern possible with the hottest assemblies in the center and colder assemblies in the periphery, see Figure 33.

Figure 31. Surry 15 x 15 PWR fuel assembly (side view left, cross section right)(EPRI, 1987b)

Figure 32. Predicted Axial Decay Heat Profile(EPRI, 1987b)

Figure 33. Spent fuel load pattern

The exterior of the cask was instrumented with thermocouples (TC) and radiation dose sensors, whereas the interior had 14 attached TCs between the basket and the cask. Finally, additional thermocouples were introduced through the top lid and into the guide tubes of the fuel assemblies. In Figure 35, the location of the exterior thermocouples (type J TC) is represented on a side and top view. Figure 34 shows the position of the interior TCs, a schematic look at a TC lance and which guide tube is used in each assembly. In total the interior basket and cask had 14 type k TC, whereas the 7 fuel assemblies measured, had 54 TCs.

The uncertainty in the temperature measurements was estimated as $\pm 4^{\circ}\text{C}$ as the lower bound, nonetheless the temperature difference measured in the mirror image and the results from the contemporary experiment on the CASTOR-V/21 suggest that the uncertainty is closer to $\pm 6^{\circ}\text{C}$ as is discussed in (Pacific Northwest Laboratory, 2018b), this upper value will be used for the TN-24P.

Figure 34 Interior thermocouple locations (EPRI, 1987b)

Figure 35. Exterior thermocouple locations (EPRI, 1987b)

With the fuel loaded and the experimental set up, 6 experiments were conducted, including the testing of three filling gases and two positions of the cask were tested. The three filling “gases” were nitrogen, helium, and vacuum, all three fillings were tested both in the horizontal and vertical position.

The experiment found that the heat transfer performance of the cask was exceptionally good with measured PCT of 232 °C for nitrogen, 214 °C for helium and 278 °C for vacuum. The experiment had conclusions and recommendations regarding cask handling and loading, heat transfer performance, COBRA SFS heat transfer analysis, shielding performance and fuel characterization and integrity.

5.5.1.1 *Limitations on the model*

As was shown in the previous section the experiment provided a very thorough overview of the experimental set up and conditions on which the experiments took place. Nonetheless there are areas where the documentation is lacking, whether that is because the information is proprietary or the authors of the public report simply did not think it was important or both. It is worth exploring them, how they have been tackled and how they may affect the end results.

The geometry is probably one of the key areas where information is lacking the most, although the general sizes of the cask are known (heights, diameters, etc.) some details are unknown. The CAD model was constructed based on the information provided in (EPRI, 1987b) and also using the example provided in the code COBRA SFS (Pacific Northwest Laboratory, 2018b) (one of the examples provided in the code is a TN-24P model, which includes a geometry description). The regions where the information is not provided are the lower plenum and the neutron shield.

What is missing from the plenum is the shape of the lower basket, and how it sits on top of the lower lid. Usually, the lower part of the basket has holes shaped like a gated shape Figure 36 (left), to let water flow through during drainage, and let the helium move during storage. Unfortunately, the actual size and shape of these “gates” is not provided in the literature, therefore the lower part of the basket was sliced off, Figure 35 right.

This modification was expected to modify the thermal behavior to a certain point, mainly in the thermal conduction of the basket to the lower lid. By lowering the heat transfer to the bottom lid means that the simulation would have lower temperatures (in the lower parts of the model) slightly higher temperatures in the rest of the model, and the temperature profile of the fuel elements would be more pronounced. As the conduction of the basket is increased, the temperature curve of the fuel assemblies flattens and homogenizes. Unfortunately, in the data for the vertical helium test, the temperatures of the TC at the bottom of the lower lid are empty (no temperatures were reported), therefore it is difficult to know the exact impact this simplification may have.

Although the heat transfer mechanism is lowered to the bottom, this region is quite far from the hottest region of the fuel assemblies (PCT approximately at 2.7 m height), and considering that the inner diameter of the cask is just 1.455 m, means that the thermal resistance through the basket to the sides is significantly smaller than to the bottom especially when considering that the contact area between basket and cylinder is roughly 3 times larger than the contact between basket and lower lid. Due to the working pressure of the TN-24P, convection barely plays an important role in the total heat transfer, therefore the modification is not expected to have any significant impact on the cooling of the cask. The results of the simulations in the lower parts do not show discrepancy with the experimental results which is why it is likely that the impact predicted initially is significantly smaller.

Figure 36. Gated lower plenum (left) and approximation used for the TN-24P model (right)

The neutron shield, as was explained in TN-24P, is a composite body made of a steel structure filled with neutron shielding material and copper fins in a radial configuration similar to Figure 14. The exact configuration of these bodies is not provided (neither is material of the neutron absorbing material, it is a borated resin, but material properties are unknown). Therefore the simplifications to the neutron shield as outlined in Model creation and best practices could not be calculated, instead the thermal conductivity of this body is taken from the (Pacific Northwest Laboratory, 2018b) where a constant value is provided to this component.

Another key information that is lacking is precise drawings of the fuel assembly, in this case the model was simplified to just the fuel clads, as will be explored in Results, this simplification is able to accurately predict the temperature distribution inside the cask in steady state simulation (for unsteady simulation the extra material might be required to be taken into account).

Another important aspect that is extremely limited in the documentation is the actual position, and localization of the cask during the test and the conditions of the laboratory. Based on the information provided it seems the test was either carried out in the warm shop or in the hot shop Figure 37. Unfortunately, the lack of these details means that the model cannot take into account whether the cask is near a wall that would affect homogeneity of the temperature profile and heat transfer coefficients, or from where the air may come. These effects could change the behavior of the outside model, nonetheless since there is no information available, the outside model took into consideration the height of both rooms and considered that the cask was far away enough from a wall so as to not skew the symmetry of the problem.

Figure 37 Laboratory.(EPRI, 1987b)

The final simplification is the thermal conductivity of the different components, although the value is known thanks to (EPRI, 1987b; Pacific Northwest Laboratory, 2018b), the exact properties of the material are unknown, therefore the material properties for the solids will remain constant in the simulation.

5.5.2 Dry Cask Simulator

The Dry Cask Simulator (DCS) was built at Sandia National Labs (SNL) in Albuquerque, New Mexico, USA, to produce validation-quality data for vertical dry cask. The DCS experiments came to be due to a need to understand the thermal-hydraulic properties of dry storage systems for commercial spent nuclear fuel in high burnup fuel (>45 GWd/MTU), due to concerns regarding cladding integrity. After the experiments were conducted a validation exercise took place.

The validation exercise was carried out using the data obtained from the dry cask simulator, five modelling institutions were granted access to the data (the NRC, the Pacific Northwest Laboratory (PNNL), Centro de Investigaciones Energéticas, MedioAmbientales y Tecnológicas (CIEMAT), and ENUSA, S.A., S.M.E with Universidad Politécnica de Madrid (UPM)).

Two configurations were used in the DCS simulating an aboveground configuration and a belowground configuration Figure 38. Most commercial dry cask in use today use are storage above ground, although in some places the belowground is used. The experiment was set up so both configurations could be considered.

Figure 38. Aboveground configuration (left), belowground configuration (right) (Lindgren and Durbin, 2017c)

The experiments conducted in the produced 40 unique data sets, fourteen sets for the above ground configuration, with power ranges from 0.5 to 5 kW, and pressures between 0.3 to 800 kPa (another 14 data sets were produced for the below ground configuration, and 13 with the cross wind machine). The two configurations can be seen in Figure 39, alongside the facility where testing took place, in this study and for the validation exercise only the aboveground configuration was used.

Figure 39. DCS configurations and CYBL facility (Lindgren and Durbin, 2017c)

The DCS consist of a dummy 9x9 BWR fuel assembly with partial length assemblies. The dummy fuel assembly and the channel box were enclosed in a carbon steel basket that represents the typical basket in a dry cask. All these components are then placed inside a pressure vessel or canister, then all components are placed inside and outside shell that allows air to flow through the air inlets to the air outlets. In Figure 40 the construction of the DCS, the top four images are of the canister and fuel assembly, and the lower two from the outside shell without the air inlets (Lindgren and Durbin, 2017c). All the component's materials were specified, with the relevant thermal properties available including the emissivity of each body.

Figure 40. DCS construction (canister and basket top four images, outside shell two bottom images)(Lindgren and Durbin, 2017c)

The temperature was captured throughout the different bodies using a number of TC, in Figure 41 the placements of TC in the fuel assembly (axial and radial TC), the channel box, basket, canister and outside vessel are presented (only one of the faces is shown in the image, for the whole TC placement (Durbin and Lindgren, 2017a)). This wide coverage allowed the researchers to gather a very throughout temperature profile in all the components of the cask. Clad temperature was measured using type k TC, the maximum expanded uncertainty in the measurements is ± 7 °C.

Figure 41. TC placements on the Fuel Assembly, Channel Box, Canister and Outside Vessel respectively (Durbin and Lindgren, 2017a)

The air mass flow into the outside shell was calculated using anemometers at the air inlet after the honeycomb structure. The honeycomb structure ensured stable and repeatable measurements at the air inlet by aligning the flow in the desired direction while introducing the least amount of pressure drop possible. The hot wire anemometers used were TSI models 8475 and 8455. For the aboveground configuration, the hot wires were fixed in the center of the inlet ducts and subjected to known mass flow rates, the output was then correlated to the forced mass flow rate input. This was coupled to a calculation using the velocity profiles along short dimension of the center of the inlet (the results were calculated with a density reference of 1.2 kg/m^3 (air at 21.1°C and 101.4 kPa , for reference the air pressure in Albuquerque is around 84 kPa). In Figure 42, the hot wire positioning and where the velocity profiles were taken.

Figure 42. Hot wire anemometer and honeycomb position (left), velocity profile calculated (right) (Durbin and Lindgren, 2017a)

5.5.2.1 Limits on the model

Unlike in the case of the TN-24P most information regarding the experiment set up was available, reducing the number of hypothesis or simplifications needed. Most of the simplifications introduced were selected by the user, not forced by the lack of information. The only change that was due to lack of information was the geometry of the bottom header and how it was attached to the rest of the fuel assembly; the bottom header used during the experiment was bought from a commercial supplier and the engineering drawings were not available. The bottom nozzle used in one of the DCS model was extracted from a similar BWR configuration, and it was attached to the channel box directly.

6 Results

In this chapter the simulation results are presented. The chapter is divided in different sections: section 6.1 and 6.2 will show the results for the TN-24P container and the DCS experiment respectively, which are used as validation for the methodology. Both cases will follow a similar structure starting with the selected boundaries and numerical scheme, how they have been determined, then the GCI to show the numerical uncertainty, and finally the different studies carried out within a cask (turbulence, gaps). These two first chapters are meant to test and validate the methodology; the first chapter will use the TN-24P with an exterior and interior model to test the coupling of the simulations, and temperature distributions both for the outside and inside. The second chapter will use the results from the DCS experiment to test different approximations to fuel assembly, like the use of spacers or headers and how changes to both pressure and heat output modify the temperature distributions.

Finally, the later sections will show the results of the extended methodology with section 6.3 showing the application of the methodology to a multiphase drainage case, 6.4 a storage facility, and finally section 6.5 will show a mechanical analysis

6.1 TN-24P

In this section the results obtained from the TN-24P cask will be shown, as was outlined in the Methodology section to validate the results several steps must be taken into account. Firstly, the convergence error will be calculated through GCI and the values reported. Later, the rest of the sensitivity analysis will be shown including the turbulence modelling, the study of the impact of the gaps and finally a new method to couple the interior results to the exterior.

6.1.1 Numerical scheme, geometry, and boundary conditions

Choosing the correct numerical scheme and selecting correctly the boundary conditions is one of the key pre requisites to ensure the quality of the simulations. As was explained in the chapter Core Methodology the methodology is divided into two coupled simulations, an outside model, and interior model.

Figure 43. Small room geometry

The exterior model consists of the cask, from the inner wall of the canister, the surrounding box of air (4x4x15 m), Figure 43, and the concrete floor on which the cask is sitting on. The size of the surrounding air and concrete floor have been chosen to ensure the boundary conditions are far enough as to limit the impact on the results, but close enough to reduce the volume of space around the cask to calculate (and therefore to reduce the computer cost). Nonetheless, to ensure that the impact was limited, another simulation was run with a larger room (15x20x15 m). The results from this model showed limited changes both in terms of temperature and heat transfer mechanisms. On Table 6-1 the results for the large and small room are presented, as can be seen both the average results (temperature and heat transfer coefficient), and the local results (maximum temperature), are nearly identical.

Table 6-1. Results for the small room and the large room

	Surface Weighted Average Temp (K)	Maximum Temp on the neutron shield (K)	HTC Weighted (W/m²·K)	Radiation (%)
Large room (15x20x15 m)	337.74	344.89	9.33	38.88
Small room (4x4x15m)	336.8	345.6	9.86	39.67

On Table 6-2 the physical and numerical scheme of the exterior model is shown. The model is a steady state calculation, the ideal gas model is used to calculate the density of the gas, the thermal properties of air were taken from (Incropera et al., 2013). The radiation model selected was the Surface-to-Surface model. This radiation model works when only when the medium (in this case air or helium) is non-participating, which it is the case for the temperature range of both models. Several turbulence models have been tested and the results will be discussed in section Turbulence modelling.

Table 6-2. Physical and numerical scheme

Pressure-velocity coupling	Coupled Flow and Energy
Discretization	2 nd Order
Temporal discretization	Steady State
Gas model	Ideal Gas
Thermal properties	Variable with temperature (when possible)
Turbulence modelling	Sensitivity analysis
Radiation	S2S

Since the exact environmental conditions of the TN-24P experiment (Experiments) were unknown, the boundary conditions have been selected as if the cask is in an open space with no walls near the cask. The four lateral walls of air are stagnation inlets, the top is a pressure outlet, this way the air can move freely. The air temperature is fixed at 20 °C (EPRI, 1987c), the lower face of the concrete is fixed as constant temperature boundary condition at 15°C (estimated value from the available information).

The heat output was distributed in the inside walls of the cask, initially this heat output was distributed throughout the different surfaces as a constant value, Table 6-3 (a percentage of the total heat output). This distribution was initially guessed based on the inner pressure of the cask, after the first iteration with the inner model. As will be explained in New method of coupling the , this method will be modified so that instead of using constant values, the heat flux is extracted directly from the interior model.

Table 6-3. Heat output distribution

Region	Percentage of heat output (Old Method)	Percentage of heat output (New Method)
Lateral cylinder	92%	93.6%
Top lid	6%	4.5%
Lower lid	2%	1.8%

The interior model consists of $\frac{1}{4}$ of the TN-24P model, Figure 44. The numerical scheme is the same as in the exterior model and can be found on Table 6-2.

Figure 44. Interior model of the TN-24P

The inner boundary conditions are the inner walls of the clads, and the outer boundary conditions are the exterior part of the neutron shield and canister. The symmetry sides were configured as symmetry planes (adiabatic and slip wall conditions), both for the solid regions and fluid regions. The heat output has been introduced as a heat flux in the inner surface of the walls with its corresponding heat output and distribution as shown in Figure 45. The guide tubes (21 per assembly) were also modelled and they have no heat flux.

Figure 45. Heat output per assembly and distribution (EPRI, 1987c)

The outer boundary conditions were taken from the exterior model as was outlined in section Interior and exterior model. The boundary condition for the regions in contact with the outside air were an *Environment* boundary condition, where both convection and radiation are taken into account. The bottom part of floor of the cask was at fixed temperature, as mentioned previously. Initially the values for the heat transfer coefficient and temperatures were extracted from the exterior model and then the height dependent values averaged and introduced with a polynomial curve.

Although this method gave accurate and viable results, latter iterations of the methodology mapped the results directly from the mesh of the exterior model into the interior mesh, skipping the averaging step, while also improving the coupling. For a single cask model, the difference between coupling the simulations though direct coupling or averaging the results is small and will be discussed in the results section. This small difference is due to the exterior results of a single cask being very homogeneous, however if the problem to solve were to be more heterogeneous, for example if there are other cask nearby, this method allows for more accurate results. Figure 48 shows the height dependent value of the heat transfer coefficient (left) and on the right the same heat transfer coefficient on the 3-D surface, in this case the 3-D distribution is very homogeneous, but by averaging the results some localize regions loose precision for example the upper and lower parts of the neutron shield.

Figure 46. Heat transfer coefficient on the neutron shield, heigth dependant value and 3-D distribution

The experimental measurements, as was explained in TN-24P, were obtained using thermocouple lances (each lance had several thermocouples at different heights). Figure 47 shows the location and naming convention that was used for the experiments and that will be used throughout this work.

Figure 47. Thermocouples in the inner part of the TN-24P (EPRI, 1987c)

6.1.2 Grid Convergence Index

As was outlined in Grid Convergence Index, the GCI allows the user to study the numerical error and reported it in a precise manner. This study is presented separately, with the results from the exterior model being presented first, then the results of the interior model.

As was mentioned in Grid Convergence Index, the grid refinement ratio should be kept constant if possible. In this case, since the air surrounding the cask is a single body and it was meshed in a single operation, it was possible to keep the refinement ratio relatively constant. The number of cells in each refinement can be found in Table 6-4. In Figure 48, the fine exterior mesh can be found, the blue region is the air region and the white region is the solid region (both the different bodies of the cask and the concrete floor). In all three cases the boundary layer on the cask surface has been kept as similar as possible so that the wall functions (both for heat transfer and turbulence) used are the same through the different meshes.

Table 6-4. Exterior meshes

Mesh	Number of cells
Coarse (3)	2463122
Fine (2)	5586033
Very fine (1)	12827695

Figure 48. Exterior mesh

The variable chosen to evaluate the GCI was maximum temperature in two of the surfaces: the neutron shield side and the top lid. These surfaces were chosen because most of the heat transfer take place through them. In Table 6-5 the results for the GCI are shown, the results show small values for the GCI, suggesting small grid size sensitivity.

Table 6-5. GCI exterior model

Region	GCI2-3 (100%)	GCI1-2 (100%)
Neutron Shield surface	0.30	0.09
Top lid	1.08	2.15

Unlike in the exterior model, the interior model is significantly more complex, and the refinement ratio could not be kept constant, in this case the refinement was performed in the fluid region and the clads. In Table 6-6 shows the number of cells for each refinement model. In this model the “Very FineZ” and “Very FineXY” are further refinements of the assembly regions (fluid and solid) the first one is a further refinement in the axial direction (100 axial divisions), and the second one a refinement in the radial direction. Figure 49 shows part of the mesh of an assembly, on the left the fine mesh, and on the right the very fineXY mesh. The idea behind studying separately the axial and radial refinements was to see the impact that each has on the convergence criteria.

Table 6-6. Inner meshes

Mesh	Number of cells
Coarse (3)	4294705
Fine (2)	6730996
Very fineZ (axial)	9537995
Very fineXY (radial)	11891116

Figure 49. Fine mesh (left), Very FineXY mesh (right)

In Table 6-7 the results for the GCI for the different assemblies can be found divided in axial or radial meshes (depending on whether the refinement was on the axial or radial direction). The three assemblies are shown along the naming convention on Figure 50. In general, the results show small convergence errors, with slightly higher values for the radial profile than the radial one, this is likely because conduction is significantly more important than convection (at this pressure), therefore the higher radial resolution gives higher numerical error.

Table 6-7. GCI inner simulation

Region	GCI23 (100%)	GCI12 (100%)
D1(Axial)	1.37	0.32
D1 (Radial)	0.46	0.08
D4(Axial)	0.25	0.02
D4(Radial)	1.53	0.83
D6(Axial)	0.38	0.07
D6 (Radial)	3.45	2.57

Figure 50. Naming convention for the assemblies and periphery holes

6.1.3 Turbulence modelling

Due to the high Rayleigh number calculated for the exterior model ($Ra > 10^{11}$), turbulence modelling is a requirement for the exterior model. The interior model has a significantly smaller Rayleigh number ($Ra > 10^8$). That Rayleigh number is in the transition zone between laminar and turbulent flow (although closer to laminar flow). Therefore, to ensure that the impact the turbulent or laminar model had was minimal, a comparison study is provided.

To understand the impact the turbulence modelling might have on the models, a comparison between different models has been performed for both simulations (exterior and inner cask models). The turbulent models selected are from the k- ϵ family, which are a two-equation model, a laminar model for the interior cask, and finally a four-equation model that has proven to accurately measured heat transfer and temperature distributions in natural convection. As discussed in section Turbulence models, there are several reasons why these models were selected. Among them is that these models are widely used, and most CFD code have one or several implementations of these models meaning that the results presented here are replicable on other codes (the exact algorithm and implementation between codes might make the results slightly different).

The second reason is that the codes user's manual (SIEMENS, 2018b) recommends this family of turbulence modelling when heat transfer is of such importance. Other codes such as CFX's user's manual (ANSYS, 2018) recommend the use of the other families of models like k- ω , whereas STAR-CCM+ does not recommend these models for this type of simulation. Since this work has been performed in STAR-CCM+, the recommendations of the creators of the code are the ones that have been followed.

And finally, as was read in the Dry cask modeling state of the art section, the k- ϵ family, has proven to have good agreement with experimental results, while keeping the computer cost low (Zhang et al., 2007).

The models that have been tested are the AKN k- ϵ Low Reynolds model (Nagano et al., 1994b), the Standard k- ϵ Low Reynolds model (Lien et al., 1996b), the two layer Realizable k- ϵ models (two versions: the Shear Driven (Wolfstein, 1969b) and the Buoyancy driven (Xu et al., 1998b)) and finally the $\overline{v^2} - f$ model (Durbin, 1991b; Lien et al., 1998). The laminar model has also been run for the inner cask model.

The results for the different turbulent models can be found on Figure 51. The top image shows the temperature distribution on the surface of the cask and a schematic view of where the values have been extracted. The bottom right graph shows the results on the neutron shield. In general, the results show a good agreement, with most models being able to capture the temperatures values and distribution. Nonetheless the Realizable k- ϵ (Buoyancy driven) model shows discrepant values, under predicting the temperatures by up to 20 °C.

The top lid results can be found on the bottom left graph. In this case there is no clear pattern between the different turbulent models, with some models slightly over predicting temperatures. Since most models can predict an accurate temperature profile, with very little difference between most models, the exemption being the Realizable k- ϵ (Buoyancy driven), the model chosen was the Realizable k- ϵ (Shear driven) due to the good agreement against the experimental results, and faster time to convergence.

Figure 51. Temperature profiles on the neutron shield (bottom left), the top lid (bottom right), and a schematic overview of where they have been extracted

To evaluate the impact of the turbulence modelling may have on the inner cask model, a case with increased convection has been selected (in this case with adiabatic gaps between canister and basket, more on this in Gaps). This increased convection can be seen on the higher Nusselt number calculated for the steel cylinder surface. In Table 6-8, the Nusselt number for the base case (Full contact), and the convection-increased case (Adiabatic).

Table 6-8. Nusselt number

	Steel Cylinder
Adiabatic	1011
Full contact	235

Unlike the outer model simulation, the inner model presents very little difference between the different turbulent models and the laminar model, especially in the inner most assembly, Figure 52 bottom left, where the maximum difference in PCT is 5 K. The outer assembly presents slightly larger differences around 6 K of PCT, Figure 52 bottom right. It is clear that the turbulent models have little impact (as was expected), and the inner cask could be run with a laminar model which should be faster (no turbulence is resolved, therefore less equations per cell and iteration), but due to the better convergence and stability seen in some of the turbulent models, the Realizable $k-\epsilon$ (Buoyancy Driven) was selected.

Figure 52. Temperatures of the different turbulence models for the inner most assembly (bottom left), and outer assembly (bottom right).

6.1.4 Outside model results

In this section the results from the exterior model will be shown. The main objectives are to show the temperatures on the cask, the impact of the cask on the environment and finally to extract the boundary conditions that will be used on the interior model.

Figure 53. Temperature on the TN-24P

Figure 54 show the temperature on a plane and the impact that the cask has on the environment, in general the impact of a single cask on the surrounding air can be considered limited, since only the closest film of air and the plume generated show higher temperatures.

Figure 54. Temperature on a plane

As for the impact on the concrete slab, the impact of a single cask is higher, with the maximum temperatures shown in Figure 55 right. Figure 55 shows the temperature profile of the concrete at different depths (only one direction is shown). It also shows the region where the temperatures of the concrete were above the air temperature (298 K). The temperatures in

contact with the cask were higher than 343 K, temperature at which concrete dehydration starts, these temperatures were seen both radially up to 1 meter from the center, and 0.3 meters below the cask, Figure 56.

Figure 55. Temperature profiles at different depths (left), and concrete above 298 K

Figure 56. Temperature profile in a center line below the cask

Besides the temperatures on the cask, used to validate the results Figure 51, and the impact on the environment Figure 54 and Figure 55, the other result that was sought after were the boundary conditions needed for the interior model. In this case, the temperatures on the concrete slab for the lower lid and the heat transfer coefficient and temperatures of the surrounding air. As was explained in Core Methodology both the heat transfer coefficient and

the temperatures of the air needed to set the boundary conditions for the interior model are extracted from the exterior model and interpolated into the interior model. For example, Figure 57 shows the air temperatures and the heat transfer coefficient on the neutron shield. The values shown represent the whole surface; with this way of plotting, for a certain height there are multiple values. This process is done for all the surfaces.

Figure 57. Air temperature near the neutron shield and simulated heat transfer coefficient.

6.1.5 Interior model results

In this section, the results for the interior model will be presented most of the chapter will deal with the impact the gaps have on the temperature distribution on the cask.

6.1.5.1 Gaps

The initial results from the interior model showed discrepancies in the exterior assemblies that were not present in the interior assemblies, meaning the model were measuring accurately the interior assemblies but it was under predicting the temperatures in the exterior assemblies. To try to understand this behavior, several sensibility analyses were performed regarding the geometry and the uncertainty that was outline in Experiments.

The one that had an impact on the temperature distribution were the contact regions between the basket and the canister. These regions, Figure 58, (from now on will be named as gaps), are not necessarily closed, meaning there can be a gap, a space between bodies. The actual size of the gaps is uncertain, even if engineering drawings were available, and they were not, transportation, handling, and thermal expansion means that it is impossible to actually know the exact size.

Nonetheless, in order to understand the impact they may have in the thermal distribution, several simulations were performed with a thermal resistance between the two bodies, these thermal resistances simulate five possible gaps:

- Full contact: there were thermal resistance between the two bodies, meaning the conduction through the two bodies was unimpeded.
- Gaps of $2\text{e-}4$ m, $1\text{e-}3$ m and $2\text{e-}3$ m modelled as a thermal resistance.
- Adiabatic: heat transfer through these contacts was blocked. This last gap was not meant to be realistic, but to obtain the maximum temperature possible.

Figure 58. Gaps

In Table 6-9, the PCT for all five cases are shown. As expected, as the thermal resistance between bodies increases so does the PCT. The temperature difference between the two extreme cases were close to 28 K.

Table 6-9. PCT for the different gaps

	Full-contact	Gap2e-4 m	Gap1e-3 m	Gap2e-3 m	Adiabatic
Temperature (K)	479.1	487.0	497.3	501.8	507.0

The results for the five different gaps can be seen on Figure 59, the temperature distribution shown are, the inner most assembly, an assembly in the middle row and an assembly on the periphery (from top to bottom), the sketch on the left shows the assembly and the red dot shows where the guide tube for the thermocouple lance was (roughly). The simulations show accurate results capturing both the magnitude, and the shape of the temperature distribution. The gap size had less impact on the temperature distribution on the inner assemblies than on the outer ones. The outer assemblies also present less accurate behavior than the inner ones, this likely due to how the exterior boundary conditions were set up, meaning that these fuel assemblies are more susceptible to a correct boundary condition.

Figure 59. Gap impact for different assemblies

The results showed the expected behavior, with higher temperatures in the inner assemblies and lower in the outer assemblies. In all assemblies the PCT was located roughly at half height due to conduction being the prevalent heat transfer mechanism inside the cask.

The gaps have an impact beyond the temperature distribution, impacting the hydraulics of the helium, changing the mass flow through the assemblies and the outer holes and the heat transfer mechanisms balance. In order to understand the changes, the mass flow through the different assemblies and outer holes was extracted. In Figure 50, the naming convention for these regions is shown.

From Figure 60, several things were clear. The first was the small mass flow through the assemblies showing that the prevalent heat transfer mechanism was not convection. The other

interesting point was that the inner assemblies have significant higher mass flows than those in the periphery (almost double the mass flow). The change to mass flow was greater in the inner assemblies (D1, D4 and D2) than in the outer ones, in all cases the maximum mass flow was reached when the gaps were closed (full contact) and therefore conduction was the most prevalent heat transfer mechanism.

Figure 60. Mass flow through the assemblies

This was initially counter intuitive, since the thermal resistance of the adiabatic case was higher, therefore convection should play a bigger role and the mass flow should increase. In order to explain this counter intuitive behavior, a more in depth look into the movement of the helium inside the cask is required.

The helium moves upwards through the fuel assemblies due to buoyancy, increasing its temperature and reducing its density. The space between the basket and the top lid (upper plenum) allows the helium to move towards the channels in the periphery (P1 through P5). From that point, it cools and moves downward and into the lower plenum, where it enters the fuel assemblies closing the primary convection loop. Another convection loop takes place in the channels in the periphery (P2 and P4), with helium going up in the inner part of the channel due to the higher temperatures of the basket and going down in the outer regions of the channel due to the lower temperatures of the canister wall. This secondary loop happens in those channels and no in the rest due to the small area the other channels have. Finally, a tertiary loop or convection cell happens on top of the fuel assemblies. This tertiary loop happens since the fuel assemblies have no top header in the simulation, but it is unlikely that it has any impact on the temperature distribution. On Figure 61 the primary loop and secondary loop (respectively) have been represented using streamlines (the tertiary loops can also be seen on top of the fuel assemblies on both images).

Figure 61. Primary loop (left) and secondary loop (right)

The strength of the secondary loop is responsible for lowering the overall mass flow into the fuel assemblies in the adiabatic case, as the mass flow “trapped” in the loop increases, the mass flow for the main loop decreases and with it the flow into the different fuel assemblies. To see that the strength of the loop has increased from the adiabatic case to the full contact case, the velocities inside this loop were measured in Figure 63. The upward velocity and downward velocities are presented, with the maximum and average value presented for the two cases, in both cases the velocities were higher in the adiabatic case, showing that the secondary loop had increased its overall mass. This was further reinforced when the Nusselt number was extracted on the surface of the canister Table 6-8.

Most of the outer channels show a similar behavior to the one seen on the fuel assemblies, the mass flow was higher on the full contact case, than in those with a thermal resistance. Both P1 and P5 channels show the opposite pattern, where the mass flow increases in the adiabatic case, likely due to the temperature gradient between the basket and canister being greater in the adiabatic case.

Figure 62. Mass flow through the periphery channels

Figure 63. Updraft velocity and downward velocity

The temperature distribution inside of the cask is modified by the gap size due to the changes in the heat transfer mechanism. As the gap increases thermal conductivity from the basket towards the canister slightly decreases, this decrease is compensated by an increase in the heat transfer to the top lid. Although the heat transfer to the different walls does not change much, the change in the radial direction does, Figure 64. As can be seen on Figure 64 right, when the gaps were closed (full contact case), most of the heat transfer on the cask was done through the gaps: up to 69% of the total heat output of the cask (20.6 kW). This value decreases as the gap increases, reaching a value of close to 19% when the gap was $2\text{e-}3\text{m}$. This decrease is taken up by the surface of the outer channels, which can increase up to 71% of the total heat output. This increase is mostly due through an increase in radiation. It is worth to consider that the gaps are just 6.44% of the lateral area, and yet they have a significant impact on the thermal performance of the cask.

Figure 64. Heat transfer throughout the canister, and radially

6.1.5.2 Conclusions

In this chapter the methodology has been presented and validated against the experimental results showing great accuracy and giving a level of detail that cannot be obtained through other methods (sub-channel modelling or porous media).

After introducing the different numerical and physical schemes, the next section of the chapter presented the results from the GCI study, showing the convergence error. This step although

cumbersome due to the difficulty of adapting a GCI study to such complex geometries was necessary to ensure that the methodology is complete and can provide accurate results.

The next section of the chapter compared the old method and new method, and although the old method is valid since it can predict temperature distributions fairly accurately, the new method provides even greater accuracy and a level of precision that cannot be easily reproduced when using boundary conditions pre-calculated through correlations. Although in this case the model was homogeneous, both on the outside and inside, it is expected that when the methodology is used in a more challenging environment, this improved method would be up to the challenge. Finally, the impact of the gap size on the cask was studied, both the impact on the temperature distribution and on the changes to the heat transfer mechanisms on the cask.

Overall, this chapter has provided the core of the methodology and the steps taken to validate the methodology. The next steps on methodology will look into the impact of modelling the spacers grid and headers using the DCS, what happens when instead of modelling a single cask multiple casks are modelled and the impact they may have on one another, and finally the gap size will be evaluated using a Finite Elements code.

6.1.6 New method of coupling the internal and external models

As was mentioned the initial way to couple the interior to the exterior simulations was through constant values of heat flux. This approach has proved to have great accuracy and precision, but to better capture the local values a new way of coupling the interior to the exterior was developed.

In the new method of coupling the results from the interior to the exterior model, the heat flux was extracted and then re-introduced directly into the exterior mesh. Since the interior model was $\frac{1}{4}$ of the geometry, and the exterior was the whole cask, a script was developed in Python that could rotate and copy the results, so that the $\frac{1}{4}$ was turned into the whole cask. This process is valid as long as the heat load is symmetric (which in this case it was). Since the results of the exterior model change with this new method, the boundary conditions of the exterior model are then reintroduced into the interior model. In this section the results from both methods will be compared both for the outside model and interior model.

Although the change from one model to another is relatively small, one of the key differences is in the temperature distribution on the lid, whereas in the first method the maximum temperature in the cask is located there, and with a value of 92 °C, in the second method the maximum temperature on the lid was 70 °C. On the neutron shield the maximum temperature on the old method was 72 °C, whereas in the new method 79°C. The change in temperature distribution throughout the outside of the cask can be seen on Figure 65, where the left image is the old method, and the right image the new method.

Figure 65. Temperature distribution, old method (left), latest method (right)

To compare the results with the experimental results, the temperatures from two lines have been extracted, one on the neutron shield, and the other on the top lid. The results can be seen on Figure 66. The old method could predict the temperature distribution accurately on the neutron shield, but it over predicted the temperature on the top lid. The new method on the other hand, predicts better the temperature distribution on the neutron shield, being capable of measuring the two upper thermocouples correctly, and it can also capture the temperature distribution on the top lid correctly.

Figure 66. Temperature distribution on the neutron shield (left) and on the top lid (right), on the old method and in the new one

The differences are not only on the temperatures on the cask but also on the concrete Figure 67, where the old method is the image on the left and the new method on the right. The new method shows higher temperatures with a maximum temperature of 77 °C versus the old method that only has a temperature of 67 °C.

Figure 67. Temperature on the concrete, old method (left), and new method (right)

The temperature distribution on the outside of the cask for both methods can be seen in Figure 65, with the old method on the left, and the new method on the right. From this image it is clear that the heat flux distribution modifies the results, with differences both in value and distribution. For example, in the new method there are regions of higher temperatures in the neutron shield that are not present on the old method. These are due to the contacts between the basket and the canister where much of the heat transfer between the inside and outside takes place. In the previous method this local values were not represented, meaning that the new method has a more pronounced heat flux distribution locally, more concentrated in the center of the inner wall. This heat flux concentration also can be seen on the temperature profile on the neutron shield Figure 66 left, by concentrating the heat flux the final profile is more pronounced, less homogeneous and more accurate to the experimental results. The change in the results on the top lid seems to be a mixture of slightly less heat overall Table 6-3, and different distribution Figure 28.

Even though the total heat through the lower lid was lower in the new method than in the old one Table 6-3, the distribution of the heat flux through the lower lid, Figure 68 mean that the temperatures seen on the concrete slab were higher in the new method. The heat flux distribution of the new method shown in Figure 68 has been overlapped with an image of the inner cask, to show how concentrated the heat flux was in the center of the lid, and the impact of the contacts between the basket and cask wall (the overlapping was done manually, it should not be taken as a perfect representation).

Overall, the new method has shown that, even small changes in heat flux can have significant impact on temperatures, the overall results are greatly improved and therefore worth the effort of directly coupling the results instead of using constant values for the boundary conditions.

Figure 68. Heat flux through the lower lid (New method)

After the changes between the new method and old method have been shown for the exterior model, the changes to the interior will be discussed here. The main difference between the two methods was the higher temperatures predicted, this can be seen throughout the cask, from the interior face of the canister as shown in Figure 69 to a slice of the canister shown in Figure 70

Figure 69. Temperature on the inner cask Wall old method (left), new method (right)

Figure 70. Temperature on a middle height plane, old method (left), and new method (right)

The difference in the temperature profiles of the different fuel assemblies can be found in Figure 71. Although the temperatures predicted were higher in the new method, the temperature profile was identical. This means that the heat transfer mechanisms predicted across both methods were the same. Therefore, the gaps study presented were not updated to the new methodology since the conclusions would have been the same, but with slightly hotter results.

Figure 71. Temperature distribution on the thermocouple lances in the different fuel assemblies. The red dot indicates roughly which guide tube was used

6.1.6.1 Conclusions

In this chapter the new method of coupling the interior model to the exterior model has been shown and compared. Although this new method has been proven to improve the already great results of the old method, it still has some limitations, for example, the script developed only works for $\frac{1}{4}$ and $\frac{1}{2}$ of a geometry (for $\frac{1}{8}$ or similar slices it would have to be modified). Nonetheless this method paves the way for better couplings, without the need of simulating the air and cask in a single simulation, which although reduces the number of steps, it also increases the overall computer cost.

6.2 DCS

In this chapter the results from the DCS will be presented. Unlike in the case of the TN-24P, the simulations were not divided into inner and outer simulations since the experiment only had a single assembly and the air ducts were small and could be simulated in a single model. In this work four experiments were simulated, two different helium pressures 800 kPa and 100 kPa, and two heat outputs 0.5 kW and 5 kW.

The objective of these simulations was twofold: the first was to test the methodology and whether it was accurate as both the pressure and heat output changes. The second objective was to test whether modelling grid spacers or the fuel assembly headers was needed in steady state simulations of dry casks. To test this second objective several simulations will be performed for each of the four experiments, without spacers or headers, with grid spacers but no header, and finally with both grid spacers and headers. To model the spacers porous media has been employed since actually simulating spacers grid would be extremely cost prohibited. The experimental set up and the model simplifications that were employed can be found on Dry Cask Simulator.

6.2.1 Geometry

The geometrical model was constructed using the public information available (Pulido et al., 2019b). Unfortunately, as was mentioned in Dry Cask Simulator, the bottom header was bought from a commercial fuel supplier, therefore the engineering drawings were not available, and the CAD model was created from other similar BWR fuel assemblies.

Two models have been created, both models consist of $\frac{1}{2}$ of the geometry with the fuel assembly being explicit in both cases. To simulate the spacers grids the length of the helium surrounding the fuel assemblies has been divided so that the spacer can be modelled with porous media. In the simulations where the spacers are not modelled, these regions were left as the rest of the helium, Figure 72 top image shows these slices. The air region has been modelled from the air inlets, to the outlets, the latter of which have been extended beyond the external cylinder so as to facilitate convergence in the air region Figure 72 (bottom image).

The difference between the two models was the header, where in one of the models there was nothing in the lower plenum (like in the model for the TN-24P), in the other a header was created Figure 72.

Figure 72. DCS geometry

6.2.2 Boundary conditions and numerical scheme

There were four types of boundary conditions in the DCS: the internal heat power of the fuel assembly, the symmetry plane, the air inlet and outlet and the external boundary condition.

The air inlets were modelled with stagnation inlets, with the ducts modelled as porous media to simulate the behavior of the flow straightener (the honeycomb structure), the pressure drop was provided by Sandia National Laboratories.

The outlets were protruded beyond the exterior cylinder to prevent backflow through them. The pressure difference between the inlets and outlets through the interior (meaning the hydrostatic pressure) could not be equalized by introducing a pressure difference in the boundary conditions. When this was done the simulation over predicts the mass flow. Initially this was exacerbated because the outlets were flush to the exterior cylinder, but by extending the outlet regions and putting a no-slip condition on the upper surface of the outlets, the flow was stagnant if no heat flux was applied. The rest of the surfaces were selected as pressure

outlets. The temperature was selected as 298 K and the atmospheric pressure at 83300 Pa (atmospheric pressure at Albuquerque, where the experiment took place).

The exterior boundary conditions were set as a constant heat transfer coefficient (1 W/m²*K) and constant temperature (300 K), unlike in the TN-24P this was considered a good approximation since the outer cylinder was covered with a thermal insulator and its temperature was only slightly above ambient. The heat flux of the interior model was simulated as constant and introduced in the inner surfaces of the clads.

The physical and numerical scheme employed in the simulations can be found on Table 6-10.

Table 6-10. Numerical and physical scheme

Pressure-velocity coupling	Coupled Flow and Energy
Discretization	2 nd Order
Temporal discretization	Steady State
Turbulence modeling	Air: Realizable k-ε Helium: Laminar and turbulent, sensibility study.
Gas model	Polynomial in T, ideal gas for helium and air (Eric W. Lemmon et al., 2019)
Thermal properties	Helium and Air: (Eric W. Lemmon et al., 2019) Solids: (Pulido et al., 2019b)
Radiation model	S2S Emissivity: material dependent (Lindgren and Durbin, 2017b)
Wall function	Two layer All y+ Wall Treatment

The properties of the porous media on the fuel assemblies were calculated from the hydraulic test conducted on (USNRC, 2012), the BWR used in the DCS experiments was similar if not the same. The report tested different fluid flows on the fuel assemblies so correlations could be used for different flows and fluids.

6.2.3 Turbulence modeling

A turbulence modeling study was performed to assess whether the inner helium was laminar or turbulent. In this case, only the high-pressure high heat output was tested (800 kPa and 5 kW). From the previous work on the TN-24P, it was known that the lower pressure cases were not affected by turbulence modelling. This model was also chosen because its Rayleigh number (1e10) was in the transition zone between turbulence and laminar (Incropera et al., 2013). The work performed in the TN-24P also narrowed the number of turbulent models to study to one, the Realizable k-ε (Wolfstein, 1969b). The air region on the other hand had a Rayleigh number well into the turbulence region (1.35E4) therefore a turbulence model was used for all 4 experiments.

Figure 73 shows the temperature difference between the laminar and turbulent model for six axial points (corresponding to where the thermocouples were placed). The maximum temperature difference was 6 K, below the band of the expanded uncertainty (which was 7 K (Pulido et al., 2019b)). Unlike in the case of the TN-24P, in this case the laminar model was

selected. This was done because unlike in the previous case, more simulations were going to be run (14 DCS simulations vs 1 TN-24P) therefore reducing the computing time per simulation was worth a slightly less converge simulation (in all cases the simulations were run until correct convergence was reach).

Figure 73. Temperature difference between laminar and turbulent model

6.2.4 GCI

To report and quantify the numerical error due to the discretization a GCI study was performed. The lessons and methods developed for the TN-24P were applied in this study, how and where to perform the refinement, and how dense it needs to be to correctly capture the heat transfer. Figure 74 shows mesh 2 Table 6-11.

Figure 74. Mesh of the DCS

The figure of merit selected for the GCI was the same as the interior model of the TN-24P: the PCT. The results of the GCI study can be found on Table 6-12, the apparent order of convergence was 1.88, the results showed small convergence error.

Table 6-11. Number of cells in each mesh

Mesh	Number of cells
Mesh 1	5.483.259
Mesh 2	3.083.746
Mesh 3	1.561.985

Table 6-12. GCI results

GCI(2)-(1) (100%)	GCI(3)-(2) (100%)
0.27	0.09

6.2.5 Results

In this section the results of the simulations of the four experiments will be presented, as previously mentioned the four experiments simulated were for two different pressures and two heat outputs Figure 84, Table 6-13. To simplify the discussion of the results, since there were a large number of simulations, the discussion will be divided in two sections. In the first section the results from the lower powered cases will be tackle, in the second part the results of the high-powered cases will be shown. This was done because the results of the high-powered cases were significantly more complex, as the simplifications introduced in the models generated more noticeable errors.

Figure 75. Temperature distribution on the 100 kPa 5 kW (upper image) and 0.5 kW (lower image)

Table 6-13. Experiments

Experiment	Power (kW)	Pressure (kPa)
Low Power Low Pressure	0.5	100
Low Power High Pressure	0.5	800
High Power Low Pressure	5	100
High Power High Pressure	5	800

In the introduction it was mentioned that there would be 3 distinct models per experiment, those being no spacers or bottom header (like in the TN-24P), spacers modelled with porous media but no bottom header and finally spacers modelled with porous media and bottom header. In order to facilitate the discussion, the cases were named case 1 through 3, in Table 6-14 the reference for each case.

Table 6-14. Cases reference

	Spacers	Bottom tie plate
Case 1	No	No
Case 2	Yes	No
Case 3	Yes	Yes

Case 1, the simplest one and the one that has been previously tested (with PWR fuel bundles instead of BWR), includes the clads and the water tubes. This model was expected to be able to reproduce the results of the lower pressure accurately since the main heat transfer mechanism were conduction (and radiation) instead of convection and the pressure drop of the spacers and bottom header was not expected to be significant enough to modify the results.

Case 2 modelled the spacers with porous media, the rest of the model was identical to Case 1. This model was expected to show a larger difference in the high-pressure experiments since convection plays a large role therefore the pressure drop could potentially affect the end results.

Finally, Case 3 could both have an increase in temperature due to the pressure drop due to the spacers, or a decrease in temperature due to the bottom header acting as a fin to help dissipate the heat, it could also increase in some regions and decreased in others. Since no engineering drawing was available, it is possible that some errors may have derive from the use of a generic bottom header.

6.2.5.1 Low power experiments (0.5 kW)

The results of the two lowered powered cases are presented in this section. As was expected, the temperature and mass flow in both experiments was lower than in the high-powered experiments. The difference between these two experiments was lower temperatures on the high-pressure experiment, and temperature distribution and PCT position skew towards the upper parts of the fuel assembly Figure 76.

Figure 76 shows the PCT calculated in each of the three Cases its position on the axial level, and where those points were measured on the two experiments (the error bars are the temperature and position uncertainty ± 7 K for the temperature and ± 0.16 m for the position). In both experiments the simulations could accurately predict the PCT, with all six Cases falling under the uncertainty band, the actual positioning of the PCT along the axial direction showed different

degrees of accuracy, with the high-pressure experiment apparently showing better accuracy than the low pressure experiment.

Figure 76. PCT and axial level for the 0.5 kW experiments

Figure 77 shows the axial profile for both of the experiments and each of the six Cases. The results of all six Cases can reproduce the axial profile, both in terms of distribution and values. The axial profile also shows the convective nature of the high-pressure experiment versus the conductive nature of the low-pressure experiments, this will be latter explored in more detail in the high powered experiments.

Figure 77. Temperature profile 0.5 kW experiments

The results for the air mass flow can be found on Table 6-15, even though calculating air mass flow in natural convection in CFD is extremely complicated due among other things the small values (see Table 6-15), the results of the Cases were in line with the experiments.

Table 6-15. Air mass flow

Mass Flow (kg/s)	100 kPa, 0.5kW	800 kPa, 0.5kW
Case 1	0.0247	0.0220
Case 2	0.0247	0.0223
Case 3	0.0247	0.0212
Experiment (Average)	0.0264 (± 0.0015)	0.0221 (± 0.0015)

Although globally the results from the different cases were similar, there were differences locally, for example in the lower parts of the fuel assemblies where the impact of the spacers and bottom header could be seen both in terms of velocities Figure 78 with an increase in velocity due to the bottom header Case 3 but lower velocities on the fuel bundle compared to Case 1.

Figure 78. Velocity magnitude (m/s) 800 kPa 0.5 kW experiment for all 3 Cases

Overall, the three Cases could reproduce the steady state temperatures on the DCS for both experiments, therefore choosing one way to model the fuel bundle over another is more a matter of preference and ease of set up and use. In this way Case 1 is the best choice, it is the easiest one to implement, and it is not prone to user errors when calculating the porous media.

6.2.5.2 High powered experiments (5 kW)

As was alluded before the high-powered experiment's simulations were significantly more complex, in that the simplifications performed showed a more pronounced impact than in the

low powered cases. The naming convention for all three cases are the same as in the previous experiments, as reflected in Table 6-14.

Figure 79 shows the axial position and value of the experiments and the simulations, like in the previous chapter the error bars are the uncertainty regarding both the position and value of the PCT (± 7 K for the PCT and ± 0.16 m for the position). It may seem that the simulations of the 800 kPa 5 kW experiment were more accurate than those at lower pressure, but this was more a factor of looking at a single data point, instead of the temperature distribution along the axial length which will show a different perspective. Nonetheless if PCT and its position were the only requirement, the three Cases in the 800 kPa 5 kW experiment could reproduce the position fairly accurately, as for the PCT value, only Case 1 was accurate, with the other two cases under predicting the temperatures. In the 100 kPa 5 kW experiment, only Case 1 could reproduce the PCT and its position, with the other two Cases under predicting the temperature and over predicting the position.

Figure 79. PCT and axial position for the 5 kW experiments and simulations

The temperature distributions along the axial length can be found on Figure 80. As was mentioned before, the axial profile of the 800 kPa 5 kW experiment's simulations showed a less accurate profile with the temperature values for all three Cases under predicting the temperature almost the entire axial length. It was only near the top and the bottom where the temperatures were similar to those of the experiment (as was shown previously with the PCT position on Figure 79). On the other hand, the 100 kPa 5 kW experiment's simulation showed great accuracy for Case 1 both in terms of the shape of the profile and the values, the other two Cases under predict the temperatures in some points by up to 40 K, a significant discrepancy.

On Table 6-16 the results for the air mass flow for all the Cases can be found, in general the values for the high-pressure experiment were accurate in all three Cases, whereas in the low pressure experiment, the air mass flow simulated was slightly below that of the experiment.

Generally, the results for the four experiments showed that Case 1 was simplification that could better capture the temperature distribution and magnitude even though it was the simplest one of them all. In the next section the reasons why the other Cases may had inaccuracies will be explored.

Figure 80. Temperature distribution along the axial length

Table 6-16. Air mass flow

Mass Flow (kg/s)	5 kW 100kPa	5 kW 800kPa
Case 1	0.0261	0.0587
Case 2	0.0262	0.0593
Case 3	0.0253	0.0572
Experiment	0.0221(±0.0015)	0.0660(±0.0015)

Porous media and spacers

To understand the previous results, it is necessary to understand what happens when the spacers were modelled with porous media and the impacts this has on dry cask simulation.

The impacts on the fuel assembly are two-fold, with the first being the pressure drop introduced in the helium path, and the second one being the change in the thermal conductivity of the porous region. Of these two impacts only the first one was intended were as the other was a byproduct of the way STAR-CCM+ (SIEMENS, 2018b) models thermal conductivity.

To better understand the effects of thermal conductivity of the porous media on the temperature distribution the results for the 100 kPa 5 kW have been employed, since conductivity plays a predominant role in the heat transfer mechanism. As can be seen on Figure 80 (right), the temperatures of Case 2 were lower than those in Case 1, even though the spacers in Case 2 should decrease the convection in the simulation, and therefore an increase of temperatures, even if a slight increase. What happened was the opposite with Case 2 being cooler than Case 1 due to the presence of the spacers, Figure 81 shows the axial profile of an entire clad for both Case 1 and Case 2. The lower temperatures of Case 2 were due to the higher thermal conductivity on the porous regions 15 higher than the surrounding helium (0.25 W/mK for the helium and 3.6 W/mK for the porous media). These regions of high conductivity not only affect the temperature distribution locally, but also globally lowering the temperature from the first spacer on, this effect can be seen clearly in the upper parts of the fuel assembly where the decrease in temperature was more dramatic. Although in reality these regions may dissipate heat better than the rest of the fuel assembly, it is unlikely that it would be as efficient as these simulations.

Figure 81. Temperature with (Case 2) and without spacers (Case 1)

To see whether the pressure drop would have an impact on the temperature distributions without the unrealistic thermal conductivity, two extra cases were run: Case 2B and 3B. These Cases were identical to Case 2 and 3 respectively but the thermal conductivity of the porous regions was modified so as to be that of the surrounding helium.

The temperature axial profile of these extra two Cases can be found on Figure 82. In both Cases the results greatly improved with the values of Case 2B being near identical to those of Case 1 and in line with the experimental results.

The bottom tie plate impact on the overall temperature distribution can be seen on Case 3B, with the temperature distribution being lower than Case 1 and the experiment in the lower regions of the fuel assemblies around 8 K. At this pressure (100 kPa) the bottom tie plate seems to be working more like a fin, whereas at higher pressures (800 kPa) the decrease of mass flow into the fuel assembly meant higher temperatures Figure 83 at the bottom of the fuel assembly.

As previously mentioned, the lack of engineering drawings was probably the reason behind the lack of accuracy of Case 3B, not only the geometry of the bottom tie plate was not the one in the experiment but also on the way it connects to the rest of the fuel bundle. It is likely that the lack of information may have meant that the contact between bottom tie plate and the channel box was not correctly modelled in the CAD and therefore the heat conduction to the lower parts of the fuel bundle increased. Nonetheless, these simulations were useful to understand how a tie plate may affect the thermal behavior and show that for steady state models it may be unnecessary to include the bottom tie plate in the model.

Figure 82. Axial temperature profile for Cases 2B and 3B

Figure 83. Axial temperature profile in Case 3B

6.2.5.3 Heat transfer mechanism

In this last section the heat transfer mechanism for each of the four experiments will be explored. To understand how the change in pressure, heat output and simplifications modify the heat transfer mechanisms the percentage of each mechanism was extracted.

The convection was measured as convection net gain taken as the total gain between the inlet and the outlet of the fuel assembly meaning that all convection that may take place inside the channel box was measured in one of the other mechanisms. This was done to simplify the calculation itself, and because the values that were wanted were global, meaning the behavior of the whole bundle was sought after not the local behavior. The values for conduction and radiation were measured in the inner surface of the channel box Figure 84. Table 6-17 through Table 6-20 shows the percentage of each heat transfer mechanism for each of the experiment and Case.

The lower pressure experiments 100 kPa Table 6-17 and Table 6-19 (0.5 kW and 5 kW respectively) showed negligible convection, with all Cases below 1%, this explains why Case 2B was identical to Case 1. Both experiments (and all Cases) showed conduction as the primary heat transfer mechanism, with the main difference between the two heat output power levels being the equilibrium point between radiation and conduction. Whereas in the 0.5 kW the equilibrium point was greatly in favor of conduction, in the 5 kW radiation plays a bigger role (although still smaller than conduction). In general, at both power levels conduction was higher in the cases where the spacers were modeled (Cases 2 and 3), but when the conductivity of the spacer was lowered to that of the surrounding helium (Cases 2B and 3B), the values of the conduction were similar to that of Case 1.

As for the 800 kPa experiments Table 6-18 and Table 6-20 (0.5 kW and 5 kW, respectively), convection played a bigger role, although the helium did not move significantly faster than in the lower pressure experiments, the higher density at 800 kPa meant stronger convection (around 400 K the helium density at 800 kPa is 0,96 Kg/m³ whereas at 100 kPa is 0,12 Kg/m³ (Eric W. Lemmon et al., 2019)) . The lack of spacers in Case 1, means that convection was higher than in the cases where the spacers were modeled (Cases 2, 2B and 3). Like in the low pressured models, radiation was more important the higher the temperature was.

Figure 84. Boundary conduction heat flux upper channel box (100 kPa 0.5 kW)

Table 6-17. Heat transfer mechanism 0.5 kW 100 kPa (%)

	Net convection (%)	Conduction (%)	Radiation (%)
Case 1	0.95	83.88	15.17
Case 2	0.03	90.59	9.38
Case 3	0.60	89.65	9.75

Table 6-18. Heat transfer mechanism 0.5 kW 800 kPa (%)

	Net convection (%)	Conduction (%)	Radiation (%)
Case 1	61.63	32.12	6.25
Case 2	44.21	50.47	5.31
Case 3	46.99	47.05	5.96

Table 6-19. Heat transfer mechanism 5 kW 100 kPa (%)

	Net convection (%)	Conduction (%)	Radiation (%)
Case 1	0.03	62.55	37.41
Case 2	0.04	73.15	27.20
Case 2B	0.00	63.14	36.80
Case 3	0.54	71.02	27.31
Case 3B	0.53	62.83	36.40

Table 6-20. Heat transfer mechanism 5kW 800 kPa (%)

	Net Convection (%)	Conduction (%)	Radiation (%)
Case 1	46.26	34.44	19.29
Case 2	30.38	51.90	17.72
Case 3	32.43	50.73	16.84
Case 3B	35.82	42.84	21.33

6.2.6 Conclusions

In this chapter the impact that modelling the grid spacers as porous media, and modelling a bottom tie plate have been presented, it has been shown that for steady state simulations both are not required in order to obtain accurate temperatures.

At lower heat output (0.5 kW) the simulations predict the PCT and the temperature distribution independently of the simplification. It is unlikely that the same would happen in unsteady state simulations, where the heat capacity of the bottom tie plate and spacers might need to be considered (therefore Case 3 or 3B might be required). The recommendation therefore is that as long as only a steady state solution is required, Case 1 (model in which only the claddings are modeled) is the best option, it is the simplest one to set up and requires less data to create the model, which is an advantage when the detailed information is not accessible.

The higher power cases (5 kW) present a more difficult challenge and the simplifications taken to model the fuel bundle show higher impacts. Nonetheless, some of the behaviors seen in these experiments are not expected to occur in a real dry cask; 5 kW is a higher output power than the ones usually extracted from the spent fuel pool (maximum heat output capacity is around 1,25 kW) , but it also surpasses the safety limit of 400 °C. However, these cases have proven very valuable to gain a better understanding of the impact's certain simplifications like the thermal conductivity of the spacers introduce. In these cases, the recommendation is the same as the one for the lower powered experiments, which is to use Case 1, the simplest case that proved the most accurate overall.

Thanks to the experimental results, the methodology has been validated, and the different simplifications employed to model the fuel bundle explored. Although the relationship between pressure and convection, and temperature and radiation inside a dry cask is not new, these models present further evidence and understanding of these relationships and how one may make further simplifications or more importantly, use the knowledge to improve thermal calculations of nuclear spent fuel.

6.3 Drainage process

The work that started in the Degree Thesis was improved and taken further in the Master Thesis named “Análisis térmico del proceso de secado y almacenamiento de un contenedor de combustible nuclear gastado con CFD” (Benavides, 2016) (Thermal analysis of the drying and storage process of a nuclear spent fuel dry cask using CFD). In this work several studies were conducted for the ENUN 32. Among these studies the results for the interior and exterior of the cask were investigated to provide information on the storage state of the cask after it is loaded with fuel assemblies, Figure 85 shows the results for the exterior and interior models.

Figure 85. ENUN 32 Exterior and interior models (Benavides, 2016)

After obtaining a “storage state” solution, the steps before that are done before the storage phase would be simulated, these steps are outlined in Dry cask loading, these include a simplified drain process, a simplified vacuum process and the heating process.

The first of these steps is the drainage of the cask, this was initially modeled with $\frac{1}{4}$ of the geometry. To model the water and helium, the multiphase model Mixture was used. The initial results showed strange behavior in the way that the water was draining out of the cask, with the central assembly draining significantly faster than the rest of the cask. Figure 86 (left) shows the water fraction of the cask, initially it was thought that the mixture model might be responsible for this behavior, but after other models were tested (Volume Of Fluid) and gave the same results it showed that the mixture model was not responsible for this behavior, the geometry simplification was found to be the responsible one.

As can be seen on Figure 86 right the water flows from the “Venteo” (venting) hole to the “Drenaje” (drainage) tube, by modeling just the quarter of the cask on the “Venteo” side, the central assembly had more openings from where the water could drain, meaning that no matter what $\frac{1}{4}$ of the cask is modeled, it cannot represent the problem fully.

This staggered drain process might happen to a degree in reality, the position of the drainage hole and that the interconnections between assembly holes is just in the lower parts of the

basket, therefore it is likely that the holes near the drain will empty slightly faster than those further away (the water in the holes nearer the “Venteo” might not be able to level due to pressure drops in the basket and nitrogen that is being introduced from the “Venteo” hole).

Figure 86. Fraction of water at 3.4 seconds in the cask (left), and water flow direction during drainage (right)(Benavides, 2016)

The next step that was taken was to try simulated the full cask, unfortunately, the computer power required to run such a simulation was not available, maybe at NASA (the time to open the case was longer than 5 hours, selecting a single boundary condition was longer than 20 minutes), so another simplification was needed. The next simplification that was tested was a model of just the fluid parts of the cask, but the computer resources needed was again large enough that it could not be justified. Other simplifications were tested, like changing the position of the drainage hole and venting hole, so that half of the cask could be modeled, again this modeled proved to be too costly in computer resources.

Test on the quarter of the cask that has the drainage hole showed a huge increase in computer cost versus a case without the drainage tube (months versus days for simulating a minute of real time). This drastic change showed that the problem was the drainage tube. In particular the entrance to the tube and the drastic change in flow direction in Figure 87 a schematic representation of the drainage tube and the flow change direction. The small incision on the lower lid means that the flow has to changed directions in a small region in a very short time and space; meaning that the time step required to simulate that small region was extremely small, on the order of 0.0001 seconds, whereas the quarter without drainage tube could be simulated with a time step of 0.05 seconds.

Figure 87. Flow direction change in the drainage tube (Benavides, 2016)

With the discovery the drainage tube was simplified to a drainage hole flush with the lower lid, and the pressure head was modeled with a pressure outlet, this allowed for simulation with time steps up to 0.1 seconds, making feasible the drainage simulation. The quarter simulation chosen was the quarter with the drainage hole, and it was further simplified so that only one quarter was being drained. Figure 88 shows the volume fraction and temperatures in the fuel at 54 seconds and 120 seconds. Like it was postulated, the drain process shows a staggered water level, with the region on top of the drain hole draining faster than the other regions.

Figure 88. Water volume fraction (top images) and fuel temperatures (bottom) at 54 seconds (left) and 120seconds (right) (Benavides, 2016)

Figure 89 shows the volume fraction of the water and the temperature in a single assembly, and one of the limitations of the model. Although some conclusions could be drawn and it showed that it could be possible to model this operation, some of the simplifications meant that other conclusions were not valid, for starters there was no boiling model, meaning that water turned into vapor without boiling. Since the clads, and the rest of the components of the fuel assemblies were not modeled, the thermal inertia was not taken into account, nonetheless this work showed that more complex behavior could be simulated, but with the increase in complexity so comes the increase in computer requirements. Nevertheless, it was a very useful application to test the preliminary methodology.

Figure 89. Water fraction and temperature in one assembly at 120 seconds (Benavides, 2016)

6.4 Storage facility

Most of the work that has been shown both in the state-of-the-art section and on this thesis has been related with the thermal behavior of a single cask, but that scenario is a simplification of the actual design of a spent fuel dry repository. The reality is that cask storage whether interim in the nuclear power plant or in a central depository have more than one cask, for example Figure 90 shows the interim facility of Central Nuclear de Trillo in Spain. The fact that there are several casks in a facility means that casks are placed near one another. The proximity of one cask to another means that the thermal mechanism and the thermal performance changes compare to the one cask case. The idea behind this chapter was to find the impact of those changes.

Figure 90. Interim facility CNT (ENSA, 2014)

As has been shown in Outside model results, the two main mechanisms that cask use to dissipate heat on the outside are convection and radiation. In a storage, as the cask near one another, the number of cool surfaces to radiate are reduced and with it the efficiency of the radiation. Convection is also expected to change, the temperatures of the surrounding air should increase, but the way the air moves could increase the temperature in those casks that are more sheltered but also reduced it in those that are more exposed. This were the two main questions that were asked in this work, whether putting casks near one another would have an impact, how big of an impact, and how would heat transfer mechanism change in a storage facility versus a single cask.

Unlike in previous works where the turbulence and GCI was performed, in this work these steps were not done, the lessons learned from the previous work allowed for a good level of certainty of the mesh created and the numerical error incurred and the turbulent model selected and the time constraint when this work was done.

6.4.1 Study cases

In NUREG-1536, there are no requirements regarding the distribution of the canisters inside a facility only that “decay heat removal system will operate reliably under normal and loading conditions”. The only requirement regarding the distribution is to keep the dose below a certain value. Therefore, four distributions are outline below which were created with three different parameters in mind:

- to understand thermal performance and how heat transfer mechanism change
- to see whether is possible to reduce the footprint of the facility from the thermal point of view

- to ensure that handling the canisters (in the facility) is easy and safe, a more compact distribution may reduce the footprint of the facility but may increase the risk for the workers

To understand the impacts outlined before, several distributions were run, all of them had 12 cask divided into rows of 4. The dry cask chosen for this exercise was the TN-24P, due to the validation process done for this specific design and the existence of experimental data. The results of these distributions were compared and normalized to the results of a single cask in the same space (the same simulation that tested an increased sized for the exterior model Outside model results).

This academic approach to the study was done for several reasons: lack of public information for actual interim facilities which made impossible to study a real case and the freedom to study four different distributions. All four simulations were done in an open room of 15x20x15m of air, and 5 m depth of concrete. The cask, like in the Outside model results, was modelled from the interior surface of the canister, with the heat flux introduced in these surfaces

The four distributions (from now on Cases) are sketched in Figure 91(not to scale). The four cases can be divided into two families, a homogeneous distribution Case A and B, and a hallway distribution Case C and D, both families had a compact version (B and D), and an expanded version (A and C).

Figure 91. The four distributions used

The cask numbering and relative position can be found in Figure 92, in blue the canisters from which the results were extracted, since there was symmetry the data was only extracted from half of the casks. In both the homogeneous cases (Cases **A** and **B**) cask 11 was (practically) equal to cask 3, and 4 and 12. Nonetheless the results are provided as proof of symmetry.

Cask1	Cask 2	Cask 3	Cask 4
Cask 5	Cask 6	Cask 7	Cask 8
Cask 9	Cask 10	Cask 11	Cask 12

Figure 92. Cask numbering sequence

6.4.2 Boundary conditions and numerical scheme

The boundary conditions selected were the same that were chosen for the exterior model, nonetheless they are as follows:

- Stagnation inlet for the lateral walls of the air region (temperature = 300 K, atmospheric pressure of 101.325 kPa).
- Pressure outlet for the ceiling of the air region (temperature = 300 K, atmospheric pressure of 101.325 kPa).

The concrete region had adiabatic lateral walls and a constant temperature on the bottom surface (288 K). Each cask has a heat output of 20.6 kW (247.2 kW in total) with a distribution per surface as Table 6-3. Heat output distribution (old method). The physical and numerical scheme can be found on Table 6-21.

Table 6-21. Physical and numerical scheme

Pressure-velocity coupling	Coupled Flow and Energy
Discretization	2 nd Order
Temporal discretization	Steady State
Gas model	Ideal Gas
Thermal properties	Variable with temperature (when possible)
Turbulence modelling	Two layer Realizable k- ε Shear Driven
Radiation	S2S

6.4.3 Results

The large data set collected (five simulations, four of which had 12 canisters each) needed processing in a way that simplified the explanation, the results were averaged and normalized to the results of the single cask, this way it was easier to understand the changes, Table 6-22 shows the values of each of the studied variables for the single cask.

Temperatures are presented in two ways, a global maximum and surface weighted averaged; as for the heat transfer coefficient, only the surface weighted average is presented. The surface weighted average was calculated as follows:

$$SA = \frac{\sum_f \phi_f A_f}{\sum_f A_f}$$

Where SA was the surface weighted average, ϕ_f was the face value of the scalar (temperature or HTC) and A_f was the face area. The value for the HTC is calculated as follows:

$$h = \frac{q''}{(T_{ref} - T_w)}$$

Where h is the heat transfer coefficient, q'' is the heat flux in each face, T_w is the temperature in the wall and T_{ref} is the temperature of the local fluid (but not the temperature of the near wall cell). This value was then averaged as explained previously in the first equation. This averaging process was selected to obtain a global perspective on the amount of convection on each cask and how it compares against other distributions and casks.

Figure 94 through Figure 97 show the results from the different Cases. The images are from top to bottom the maximum temperature on the neutron shield, the surface weighted average

temperature, the surface weighted average heat transfer coefficient, and finally the percentage of radiation (the surface integral value for all outer surfaces) out of the total heat output. The first two were meant to give an idea of how the temperatures change, the other two variables were studied to see the changes in the heat transfer mechanism.

Table 6-22. Results for a single cask

	Surface Weighted Average Temp (K)	Maximum Temp (K)	HTC Weighted ($\text{W}/\text{m}^2\cdot\text{K}$)	Radiation (%)
Single	337.74	344.89	9.33	38.88

The results for the single cask on the large room (compared to Outside model results) show very little difference. In Figure 93 the temperature surface distribution shows a very homogeneous distribution, with higher temperatures on the top lid and significant impact on the concrete near the cask.

Figure 93. Temperature on the surface of a single cask

The maximum temperature reached in the different distribution was 388 K in Case B, 44 K higher than in the single cask, a significant increase. This value was reached in two of the canisters: Cask 6 and 7 (the first is not shown due to symmetry). These casks were the canisters in the middle of the distribution (as expected), since those canisters were more sheltered by the other casks than the others. This pattern of higher maximum temperatures near the center of the distribution was present in all cases, but the peak temperature reached gets lower the more dispersed the canisters were Figure 94. Case D presented a similar pattern to Case B, except cask 3 and 4, where the pattern was broken, and they followed a similar behavior to that of the dispersed Cases (A and C). What was surprising was how close the behavior of cask 7 through 12, were to that of Case C, since in Case D the gap between rows was expected to a bigger impact.

Figure 94. Maximum temperatures (normalized)

The dispersed distributions showed very little difference between them with slightly higher temperatures in Case C. Overall the dispersed models not only were cooler, but also more homogeneous, meaning that overall, most cask responded similarly.

Figure 95. Surface weighted average temperatures (normalized)

Looking at the results from the surface weighted temperatures, Figure 95, the same pattern aroused, with higher temperatures in Case B and D, and cooler temperatures in A and C. Case A presented very similar temperatures to that of the single cask. In casks 3, 4 11 and 12 the casks that were in the periphery of the distribution, it was only in the central ones where the temperature increased, this started to show that with enough space between casks the impact can be negligible. The results also showed that the maximum temperatures were considerably

more sensitive to the position of the cask and overall distribution, than the average temperatures.

Figure 96. Surface weighted average HTC (normalized)

Figure 97. Percentage of radiation

One thing that was common among all distributions was that the temperature on the surface of the cask turns considerably more heterogeneous, as can be seen in Figure 98, with great temperature differences on the same body surface (up to 30 K on the neutron shield in the **Case D** case). Although more pronounced on the compact Cases like in Figure 98, the more dispersed cases also showed greater temperature gradients up to 20 K like in Case A, Figure 99 than those seen on the single cask.

Figure 98. Temperatures on Case D

Figure 99. Temperatures on Case A

Heat transfer mechanisms also changed with distribution. When looking at heat transfer coefficient normalized, Figure 96, it was clear that the Case D had very little air flow between the canisters. The rest of the distributions were somewhat more complex, in that some canisters benefit from the increase in air mass flow, this happened in the casks 3, 4, 11 and 12 in Case C. In this case, there seemed to be a slight increase in HTC for the canisters in the periphery and worsening conditions for the canisters in the middle row, which indicate that the shielding (of the central casks) that was expected to happen, was happening. In some of the cask there was an increase HTC, especially in Case A where the casks in the periphery.

In general, it seemed that the outer casks were shielding (to a degree) the inner casks from the air flow, making heat removal harder in the central positions, but better in the exterior ones. Cask 8 in the **Case C** being the exception, probably due the fact that this distribution was open enough to not block the air to most of the casks (the inner most cask still suffers from lower air flow). This shielding can be seen in Figure 100, the tracelines are represented on a plane crossing through casks 3, 7 and 11.

Figure 100. Tracelines on Case D

The percentage of radiation out of total heat output, Figure 97, presents a different picture from that of the natural convection of the single cask. In this case radiation plays a major role in the inner casks, and a lower one on the outer casks. The values presented are the surface integral values. The main reason why most casks have lower percentage of radiation than that of the single cask was due to the fact that they themselves were being subjected to the radiation of other casks, meaning that some part of the cask was receiving net positive radiation (and this lowered the integral value). All this can be seen in Figure 101, (where warmer colors means surface radiation influx, and cooler ones means positive outgoing heat flux) the cask represented are cask 11 and 12 (left to right) on **Case D**.

Figure 101. Radiation heat flux cask 11 and cask 12 Case D

The maximum temperature on the concrete floor for the single cask was 329 K, this increased to 374 K for the Case D, 376 K for the Case B, 356 K for the Case C and 356 K for the Case A. In all cases this was a fairly large increase in temperatures, which could potentially damage the concrete.

6.4.4 Conclusions

The objective of this work was to evaluate whether different cask distributions of nuclear spent fuel in a repository could have an impact on thermal performance. The second objective was to

begin to understand the complex thermal behavior in the storage facilities so that better strategies could be develop.

Overall, it was clear that distributions that had spaced enough between the casks (both dispersed cases) or had sufficiently large space between the different rows (casks 3 and 4 **Case C**), did not suffer such a large thermal impact as those in the less spaced regions (**Case B** and inner region for the **Case D**). With this in mind, it seems that if there is enough space (exactly how much is to be determined) between casks in the same row or the rows themselves the thermal impact is very manageable, (maximum temperature from 344.9 K for the single cask and 354.8 K for the **Case C**).

In future works, the simulations presented here would need to be coupled to an inner simulation, where the impact on PCT will need to be assessed. This may prove challenging due to the heterogeneous results obtain for some of the cask where the $\frac{1}{4}$ symmetry cannot capture these changes.

Besides the coupling to the inner simulations, a more realistic storage facility will have to be simulated (whether interior or exterior), although an all open on all sides probatory case has helped us to understand the problem and see that the impact can be big enough to warrant further inquiry, a real storage facility would allow for a study with more precision.

A real storage facility will help develop casks distributions in a more realistic way (in an inside facility the air flow is more restricted and the building structure will heat up whether from the hot air or radiation from the casks, and an outside facility solar radiation will play also a role). In this work all cask have the same heat output (20.6kW), but in reality the heat output can vary significantly (burnup, time spent in the pool and load), specially throughout the live of a storage facility (20-40 years), therefore a possible way to lower the area footprint would be to move older and cooler casks to the center of the distributions, and newer and hotter casks in the periphery, ensuring an optimal thermal output without increasing the footprint or crossing the safety limits, these are some of the studies that could be carried in a real storage facility.

Another possible strategy hinted at in the results is casks orientation. Due to the heterogeneous results it seems likely that the inner part of the cask won't be symmetrical, with a very hot side on the inner faces of the distribution (both hallways simulations (**cases C and D**)) and a cooler side on the exterior. It might be possible to load the hotter assemblies on one side and orientate this side to the cooler side of the distribution, again without compromising safety regulations. This approach might not be possible, thermal behavior is not the only factor to take into consideration when loading a canister (reactivity and doses also play a role).

6.5 Mechanical analysis

As was shown in section Gaps, the gap between basket and canister can have a large impact on the thermal behavior of the cask, but due to the limitations of CFD codes, those gaps could only be realistically be studied through the use of thermal resistances. In this work the idea was to try to shed light into the behavior of these gaps by coupling the results shown in section TN-24P, to a FE code in this case ABAQUS (ABAQUS, 2017).

To the author's knowledge, this the first attempt to perform a detailed thermo-mechanical analysis of the TN-24P cask using temperatures obtained in a CFD simulation. The aim of this work was thus to improve the understanding of the gaps behavior through the detailed analyses of the thermal displacements between cask components. Additionally, the thermal displacements and stresses in the cask components were also analyzed to verify that the general safety limits were met.

To couple the results from STAR-CCM+ to ABAQUS a methodology was developed, as it was outlined in Mechanical Calculation

The structural model of the TN-24P cask and thermal boundary conditions employed in the simulations are described first, and although they were shown in previous sections, they will be repeated here so as to make reading this section easier, and to show the interpolation into ABAQUS. After this the main outcomes of the paper, which includes the individual component results as well as the results of the cask's gaps detailed analyses. At the end, the conclusions are drawn.

6.5.1 Structural model of the dry storage cask

This section presents the structural model employed in the thermo-mechanical analysis of the TN-24P cask with the ABAQUS code (ABAQUS, 2017). Additionally, the cask temperatures employed from TN-24P section were those with the gap size of 0.2 mm.

6.5.1.1 Geometry, FE meshes and mechanical boundary conditions

The geometry of the cask's components used in the CFD interior model were imported into ABAQUS to develop the structural model. The model was effectively composed of four components shown in Figure 102, namely, (i) the top and bottom lids and the steel canister, all made of stainless steel and modeled here as a single component, (ii) the neutron shield composite made of a neutron-absorbing resin, copper fins and steel, (iii) the basket made of borated aluminum and (iv) the six fuel assemblies modelled with the fuel pin claddings made of zircalloy. It is worth mentioning at this point that because the canister and neutron shield were welded together during manufacturing, these two components (also with the lids) have been modeled as a single component with the different materials assigned on the appropriate model regions. This changes with respect to the CFD model were done due to the different requirements of the two codes.

Due to the proprietary nature of the cask design, the exact material properties of the components were unknown. Therefore, equivalent materials were chosen such as the stainless steel properties from ("ASM HANDBOOK VOLUME 1: Properties and Selection: Irons, Steels, and High-Performance Alloys," 1992) for the steel components and the borated aluminum of the basket and zircalloy of the fuel assemblies from (Barnhurst et al., 1992). Equivalent material properties for the neutron shield composite were calculated with mixture rules from the

individual materials extracted from (Ashby, 2011). The material properties used in the analysis can be found in Table 6-25.

Table 6-23. Material properties of the cask's components

Material	Young's modulus [Pa]	Poisson ratio [-]	Thermal expansion coefficient [1/K]
Stainless steel	2.00E+11	0.30	1.70E-05
Borated aluminum	6.89E+10	0.33	2.17E-05
Zircalloy	9.93E+10	0.35	5.89E-06
Neutron absorber resin	1.23E+11	0.22	9.40E-06
Copper	1.28E+11	0.36	1.76E-05
Neutron shield composite	1.36E+11	0.24	1.11E-05

Figure 102. Geometry of the 1/4 model of the cask and its components in the structural model in ABAQUS

The FE meshes of individual components, shown in Figure 103 and listed in Table 6-24, consist of linear hexahedral elements (type C3D8R). These meshes were refined until the components' temperature gradients obtained in the CFD simulation were captured accurately in the FE meshes.

Table 6-24. Number of elements in components' meshes

Component	Elements
Canister (including both lids)	245719
Basket	208080
Neutron shield	88725
Fuel assembly (per assembly)	360000

The mechanical boundary conditions defined on the model components are shown in Figure 104. These include the zero displacements in the normal directions to the symmetry planes ($U_x=0$ and $U_y=0$) of the steel canister, top and bottom lids, basket and neutron shield and the restricted movement in the vertical direction ($U_z=0$) of the lower surfaces of bottom lid and the basket. The latter was a simplification due to simplified geometry of the basket developed in the CFD interior model. Similarly, the simplified geometry of the fuel assemblies as only claddings also required appropriate boundary conditions. Thus, the boundary conditions on the individual pins of fuel assemblies, also shown in Figure 104, consist of zero displacement in vertical direction ($U_z=0$) and 8 points (4 in the upper surface and 4 in the lower surface) have restricted displacements in the on-plane directions ($U_x=0$ and $U_y=0$).

Figure 103. Finite element meshes of the cask's components. Note that a short vertical section of the fuel pin assembly was shown here

Figure 104. Mechanical boundary conditions on the cask's components

The only loads considered in the analysis were the temperatures of the cask components obtained in the steady-state CFD simulation with the interior model, which employed as thermal boundary conditions. These loads were thus the source of the thermal displacements and stresses in the thermo-mechanical analysis. Other loads, such as the inner and outer pressures acting on the fuel elements, were not considered in the present study. Outer pressure is typically about 0.1 MPa while the inner pressure, highly dependent of the history inside the reactor, may be about 2 MPa at 20°C ("BENCHMARKS FOR UNCERTAINTY ANALYSIS IN MODELLING (UAM) FOR THE DESIGN, OPERATION AND SAFETY ANALYSIS OF LWR," 2013)

6.5.1.2 Thermal boundary conditions from CFD simulation

The temperatures of the cask components obtained in the CFD simulation were mapped onto the FE meshes using the analytical mapped field interpolation tool in ABAQUS. This was a very valuable tool for multidisciplinary studies, as it allows importing volumetric and surface temperature fields from external applications using ASCII files and it performs the interpolation onto arbitrary FE meshes. In the case of study, the volumetric temperatures for each component were exported from STAR-CCM+ using coma-separated values (CSV) files containing the nodal coordinates and temperatures of the CFD mesh. Each file was then imported into ABAQUS through the analytical mapped field tool and, after interpolation (or extrapolation) of the data onto the FE mesh, this was imposed as thermal boundary condition in the structural analysis. Therefore, no extra steps were needed if the FE mesh in ABAQUS is modified, making the overall process seamless. This strategy has proven to be very useful in sensitivity analyses aiming at capturing on the component's FE meshes the temperature gradients present in the CFD meshes. As mentioned previously, the FE meshes presented in Figure 103 were developed with this purpose, since the localized temperature gradients obtained in the CFD simulation may be an important source of thermal stresses.

Figure 105. Temperature distribution of the complete cask without fuel assemblies

Figure 105 shows the temperature distribution of the cask's structural components, i.e., without fuel assemblies. Radial and vertical temperature gradients dominate the overall system due to the circumferential symmetry, with the highest temperatures found in the center region of the basket.

Figure 106. Temperature distributions mapped onto the FE meshes of the (a) top lid, (b) bottom lid, (c) neutron shield and (d) steel canister with neutron shield

Figure 106 shows the temperature distributions of the components separately, i.e., both lids, the neutron shield and the steel canister. The temperature distribution of the steel canister

inner surface in Figure 106-d presents a clear example of local temperature gradients, with four narrow bands of high temperature representing the contact surfaces between the steel canister and the basket, i.e., the gaps in Figure 58. It is worth repeating here that, due to the natural convection movement of the helium inside the cask, most of the heat transfer from the fuel to the cask was found to be through conduction and radiation along these gaps Interior model. This was the reason why further understanding of the gaps behavior was considered to be relevant for the overall thermal performance of the cask. Although it did not play a main role, the effect of convection heat transfer can also be seen in Figure 106-a through the higher temperatures at the center of the top lid in contact with the helium. On the other hand, the bottom lid in Figure 106-b presents higher temperatures at the connection with the canister than at the center, region also in contact with the helium. Finally, the neutron shield shown in Figure 106-c presents higher temperatures in the middle due to conduction playing the main role inside the cask. If this was not the case, the highest temperature would be expected at the top.

Due to its proximity to the fuel, the basket presents the highest temperature of all the structural components. As shown in Figure 107, a maximum temperature of almost 200°C in the center can be expected.

Figure 107. Temperature distribution of the basket

All assemblies present somehow a similar behavior, with higher temperatures in the middle and significantly colder, about 100°C, lower parts. As expected, assemblies closer to the center of the cask were hotter than those in the periphery. Nevertheless, temperature gradients can also be found within each assembly, with the center of the assembly being the hottest part, and within individual rod claddings. As shown also in Figure 108, the region of the rod facing the center of the assembly was slightly hotter than the region facing the outer part, mostly due to thermal radiation.

Figure 108. Temperature of the fuel bundle of assemblies, of a single fuel assembly from the periphery and of a short section of a single rod cladding

6.5.2 Thermo-mechanical analysis results

Non-uniform temperature distribution implies a non-uniform deformation of a component. Typically, non-uniform temperature also means that internal constraints may evolve within the component, as neighboring sections at different temperatures preclude the free deformations of the adjacent ones. In this section, the results of the thermal displacements and stresses arising in the cask's components as a result of the thermal loads from CFD were presented in the first place. Next, the detailed study of the gaps was performed through the analysis of the relative displacements between the basket and the canister, with the aim to gain a better understanding of the gaps behavior in realistic conditions and, ultimately, improve the gaps modeling in future CFD analyses.

6.5.2.1 Component results overview

Figure 109 presents the magnitude and radial component of displacements of the canister with the lids and the neutron shield. The major contribution to the overall displacements was the vertical direction with a maximum of 2.9 mm, while the radial displacement was about four times smaller. The displacements generated by the steady-state temperatures of the cask were rather low, and not expected to be of concern for the safe operation and performance of the cask.

Figure 109. Displacements magnitude (left) and radial component (right) of the canister and neutron shield

Figure 110 shows the von Mises stress distribution in the cask and neutron shield. The highest stresses appear in the neutron shield (Figure 110-a), at the inner surface of the canister (Figure 110-a) and at the corner edge between the canister and the neutron shield (Figure 110-b). The stresses on the inner surface of the canister coincide with the four bands of localized high temperatures shown in Figure 106-d, with values oscillating from about 39 MPa to 47 MPa, as illustrated by the stresses along a circumferential path near mid-height of the inner surface of the canister (see inset graph in Figure 110). Thus, in this case, the stresses were of clear thermal origin due to local temperature gradients. On the other hand, the high stresses in the neutron shield were due to the combined effect of temperature gradients (the steel canister was hotter than the neutron shield) and the different thermal expansion coefficients of the materials. Similar causes, together with the sharp edge geometry, can also explain the high stresses along the edge between the canister and neutron shield in Figure 110b. Nevertheless, the thermal stresses were generally low, and below the typical yield strength of the materials, which, in the case of e.g. stainless steel, was about 200 MPa.

Figure 110. Von Mises stress distribution in the canister and neutron shield (a and b – deformation scale factor 700), in the canister without neutron shield (c) and stresses along a circumferential path at middle height of the inner surface of the canister (inset graph)

Higher temperature means higher displacements of the basket than previous components, which are shown in Figure 111 to reach values up to 10 mm and 2.5 mm in the axial and radial directions, respectively. The deformation in the radial direction will be discussed in the next section to study the gap behavior.

Figure 111. Displacements in the axial (left) and radial (right) directions of the basket

Figure 112 presents the stresses obtained in the basket. Stresses up to 95 MPa can be observed in the central region where the highest temperature was present (see Figure 107), at the top around the central assembly, and at the periphery edges. The stresses along the centerline of the basket, where the two symmetry planes meet, are shown in the inset graph of Figure 112. The stresses in the basket were the highest among the stresses in the cask's components. However, these were still well below the yield strength of aluminum, which is about 250 MPa.

Figure 112. Von Mises stress distribution in the basket and the stresses along the centerline (inset graph)

Figure 113 and Figure 114 present, respectively, the displacements and stresses in the fuel assemblies. The assemblies' results shown here were qualitative due to the geometry and boundary conditions simplifications in the model. Nevertheless, the overall deformation behavior and the stress levels from thermal origin can be extracted from these results. Also in the fuel, the vertical component of the displacement of almost 4 mm was the most important contributor to the overall deformation. Within one assembly, the upper region of the fuel pins closer to the central region of the cask has higher deformation than those away from the center. This behavior is, in fact, more pronounced in the assemblies further away from the center (periphery), as shown in Figure 113 (top left image), where the pins facing inwards present higher deformation than the ones facing outward.

Figure 113. Displacements magnitude of the fuel bundle of assemblies and of two individual assemblies: central (right) and periphery (left). Note the deformation scale factor of individual assemblies and that these have been rotated 90 around z-axis with respect to the fuel bundle

The stresses in the fuel assemblies presented in Figure 114 indicate that the thermal loads have a very low contribution, of about 1 MPa, to the 90 MPa limit. Reasons for this were the relative low temperatures of the fuel, as compared to the maximum limit of 400°C, with low temperature gradients, the lack of pressure loads, and other factors such as the contact between the pellet and cladding. Nevertheless, it is still worth showing that within the safe range of fuel temperatures, the stress levels from thermal origin were small.

Figure 114. Von Mises stress distribution in the fuel assemblies

6.5.2.2 Detailed analysis of the gaps

The behavior of the gaps between the canister and the basket shown Figure 58 is explored in this section.

Figure 115. Temperatures of the central assembly obtained in three CFD simulations using different thermal resistances to model the gaps versus the experimental results (Benavides et al., 2019)

As it has been previously explained, the gap size has been found to have a strong influence on the calculated PCT in previous studies. Therefore, a better understanding on their behavior under the cask steady-state conditions may help explaining the deviations between CFD and experimental measurements and also developing future CFD models, which require simplifications due to lack of precise information and high computational costs. For the analyses in this section, three sets of CFD temperatures were used (see Figure 115), each with a different thermal resistance used to model the gaps or, in other words, to model the contact between the canister and basket surfaces. The CFD temperature results include those with (i) the thermal gap of 0.2 mm employed in previous sections and that delivered the best results as compared to the experimental thermo-couple readings of the central assembly, (ii) full contact (or no gaps), delivering the lowest fuel temperatures and (iii) adiabatic (or no contact between surfaces), being the highest fuel temperature scenario.

As shown in previous sections, the canister has lower temperatures than the basket. Therefore, the gaps were expected to close, i.e. the distance between components to become smaller. The gaps can also be expected to close in a non-uniform manner along the cask's height due to the non-uniform temperatures and displacements of the components along the gap locations. Figure 116 shows the (absolute) relative displacement between the canister and basket at the C1 and C2 gap locations in Figure 58. The relative displacement can be understood also as a measure of the initial gap size required to prevent rigid contact between the basket and the canister. Note that the results for the C3 and C4 locations were equivalent due to model symmetry.

Figure 116. Relative displacements along height between the basket and canister at the C1 (left) and C2 (right) gap locations (see Figure 58)

The results in Figure 116 were in line with the temperature results in Figure 115, i.e., the hotter the components are, the larger were the relative displacements and, therefore, the larger the initial gaps needed to be to prevent contact. The two extreme models, adiabatic and full contact, show, respectively, the maximum and minimum relative displacements obtained, or the minimum and maximum gaps necessary to avoid contact. The results show a substantial difference in the relative displacement with height as well as quantitative differences between the C1 and C2 gap locations. These results were summarized in Table 6-25, which presents the maximum and average relative displacements obtained for the different gap locations and cases considered.

Table 6-25. Maximum and average relative displacements between basket and canister

	Maximum [m]	Average [m]		Maximum [m]	Average [m]
C1_contact	1.49E-03	1.28E-03	C2_contact	1.10E-03	9.62E-04
C1_0.2mm	1.64E-03	1.40E-03	C2_0.2mm	1.26E-03	1.09E-03
C1_adiabatic	2.12E-03	1.80E-03	C2_adiabatic	1.70E-03	1.47E-03

An interpretation of the results just presented from a thermal point of view was that, in the experimental canister, the gap might have been nearly closed at mid-height (where the maximum relative displacements were obtained), whereas bigger gaps remain on the upper and lower regions (where the minimum relative displacements were obtained). This hypothesis of the gap being partially closed could explain why, in Figure 115, the full contact results were cooler than the experimental results while the most accurate temperatures were obtained with a small constant gap, as the latter probably captures the global thermal behavior. Thus, future CFD modeling efforts could be directed towards implementing a thermal resistance varying with height following the results presented here.

6.5.3 Conclusions

In this study, the thermo-mechanical analysis of a nuclear spent fuel dry cask was performed using the temperature fields of the cask's components obtained in a previous CFD study. The aim of the study was to improve the overall knowledge of dry cask behavior due to thermal loads and, in particular, the behavior of the gaps between the basket and canister.

The results of the analysis have shown rather low thermal displacements and stresses in all cask components relative to the safety limits. This therefore corroborates the safe operation of the dry cask system. The behavior of the gaps has shown that these were highly dependent on height and position, thus, paving the way for improved CFD models in future studies. Finally, the non-uniform relative displacements along the height between basket and canister have also explained the observed temperature differences between CFD simulations and experiments.

7 Conclusions

The main objective of this thesis was to develop a methodology to simulate nuclear spent fuel cask using CFD and to validate it with experimental results to ensure reliable and accurate results with a competitive computational cost.

To accomplish this, it has been necessary to learn how to create the model from scratch. This process started with obtaining data from the literature, learning how to deal with the gaps in the available public information. The next big step was to create a CAD model and simplified it so that the following steps could be done with the available resources (time constraints and computer power). Probably one of the most difficult challenges when one starts working with CFD is meshing the geometry, this especially challenging in this case due to the complex geometry of the fuel assemblies and casks. This step that is now very intuitive, but developing to the level that it has now a days took many iterations and headaches. The recommendations about meshing and setting up the model found throughout this thesis are meant to help those that would tackle these problems and hopefully make these crucial steps easier.

The first step in order to validate the methodology was to simulate the TN-24P, which was done in a two-step coupled process. In the first step the exterior of the cask was simulated, to ensure that the results were valid several studies were conducted in this model. The turbulence modelling showed that most turbulent models used, could predict the exterior temperatures with accuracy. The GCI provided showed that the discretization error was small. Finally, the results showed little impact on the air temperatures surrounding the cask, and high temperatures on the concrete pad, which may damage it.

This exterior model was coupled to the interior model through the boundary conditions. The study on the impact of turbulence on the temperature distribution on the interior model showed little impact, with all models being able to predict both PCT and temperature distribution in all the fuel assemblies. The GCI showed that the discretization used on the fuel assemblies was correct, as the numerical error was small. The last study conducted on the interior was the impact of the gap size between the basket and the main body of the cask. These gaps not only had a pronounced impact on the temperature distribution (with PCT increasing up to 28K) but also the thermos hydraulics of the cask.

Initially, the coupling between exterior and interior models was done through polynomial values and averaging, meaning that the heat transfer coefficient from the interior model used on the exterior was a constant value, and the heat transfer coefficient and temperature from the exterior model was averaged and introduced as a polynomial value. This approach was accurate, but it had limitations. For example: when the heat flux was introduced as a constant value the conduction through the gaps or how the heat flux on the lower lid is concentrated in the center, could not be seen on the exterior model. By using the actual heat flux not only could these effects be seen on the exterior model, but the results from this method were even more accurate. Although this method of coupling has only been tested and compared, it will allow for more complex couplings, like on the case of a storage facility where the boundary conditions are more heterogeneous.

The second experiment that was simulated was the DCS. Unlike the TN-24P the DCS was tested at different pressures and heat outputs. The experiment measured both the temperatures and air mass flow of a single BWR assembly in a configuration similar to a WT cask. The turbulent study in this work was only performed in the high pressure case, as convection was more

prevalent, the results showed very little difference between a turbulent model and a laminar one, therefore the laminar model was chosen for the four experiments. The four experiments also allowed us to see whether the natural convection of the surrounding air was being correctly model, and the simulation results showed good agreement in all four experiments, meaning the overall heat transfer to the environment was being calculated correctly. These experiments were used to test whether the fuel representation was accurate or not. To simulate the spacers porous media was used, the bottom header was also simulated. The results showed that the way porous media models heat conduction means that it is not a good way to simulate grid spacers, and although further changing the thermal conductivity circumvented the problems, there were no advantages in simulating these components in steady state models.

Before the cask can be placed in the storage facility, the fuel inside the cask must be dry. This process is extremely challenging in terms of simulations, it is a long process in which there are multiple species and multiple phases. To try to simulate this, the simulations were divided into several steps and simplified. Although several of these steps could be simulated to a degree, the simplifications needed to reduce the computational requirements, meant that the results proved that better simplifications were needed, and significant more computational power would be required.

Up to this point all the simulations have only considered a single cask, but in reality casks are placed besides each other, meaning that the thermal performance of the casks change. In this chapter, four different distributions were tested to see the impact each distribution had on thermal performance. The results of the different distributions showed that all cask had worse thermal performance with an increase in temperatures, and in some cases with increases in temperatures of up to 44 K in the exterior. The results also showed that this could be mitigated by ensuring enough space between casks. The study also hinted at the possibility that it may be possible to place casks with lower heat output in the center, and higher in the periphery, limiting the impact to those casks that are already cooler.

The last work performed for this thesis tried to shed light into the behavior of the gaps between basket and the main body of the cask. To better understand the behavior, the results from the TN-24P, were extracted and introduced into a FE code (ABAQUS). The mechanical analysis showed relatively small stresses in all the components of the cask. The displacements of the different components were also small. More importantly they showed that the gap size was not constant but height dependent, with a rotated U shape curve. This work also highlighted the advantages of coupling different codes, since a mechanical analysis cannot be performed in a CFD code.

This thesis and all the studies that have been conducted have shown the methodology, the steps needed to ensure that the results are valid. This process starts with the planning phase and the construction of the models, for which some guidelines have been provided. Then the results have shown the advantage of a two-step coupling method to obtain, not only the results for the interior of the cask but also the exterior. This work has shown the impact that turbulence modelling can have both on the outside and in the inside. Fuel representation has also been tackled, showing that for steady state calculations, simulating the just the clads is enough. But the work presented has gone beyond the calculations of a single cask in a steady state condition. For example: showing a first try at simulating the drying process, how placing a cask near other casks in a storage facility changes their thermal behavior, and finally the mechanical analysis has tested how the gap size is, and the shape of it.

7.1 Future works

In this section the future works that have risen from this thesis will be discussed some of them are meant to improve the core methodology, whereas others are meant to use this methodology and take it further. Some of this are currently being work on, others are further away but are lines of investigation that may prove useful and interesting.

One of the limitations of this thesis was the lack of information regarding the cask, mainly in terms of material properties and geometries. A more in-depth investigation using engineering drawings may shed light into whether the simplifications used for the core methodology are enough, or if there is some aspect that is missing. For example, most basket are not a single material, but several (this was not the case for the TN-24P), this different bodies could be simulated separately or together using equivalent thermal properties. Although it seems that the top and bottom header are not necessary for steady state solutions, this may need to be tested on a whole cask instead of a single component (it is not expected to change dramatically, but it needs to be proven).

Another future work is to tackle real storages facilities, to see whether the impact we have seen on this work could be problematic in real scenario. This would include considering weather patterns, solar radiation and even accidental conditions.

One aspect that has been only briefly studied in this thesis are transient simulations and how to perform them in such a way that the computer cost is manageable. In this sense changing the properties of the clads so that they have the same thermal inertia as a real fuel rod may prove useful. If such simplifications are possible, they would have to be validated against experiments to ensure that the methodology is applicable.

If the transient simplifications are proven to be valid many works could be derived from this. One of this works would be to simulate the drying and draining of the cask. This would improve the works shown in this thesis and could potentially answer several questions regarding this procedure. Besides normal operations, with a transient methodology developed, other off normal behavior could be studied, like accidents. For example, several rods breaking and liberating fission gases, and seeing whether this could be detected by measuring the temperature outside. Other accidents to simulate could be: fire on the outside of the cask, the cask being buried by debris due to an earthquake.

8 References

- ABAQUS, 2017. ABAQUS, Dassault Systèmes Simulia Corp, Providence, RI, USA, 2017.
- Ade, B.J., Gauld, I.C., 2011. Decay Heat Calculations for PWR and BWR Assemblies Fueled with Uranium and Plutonium Mixed Oxide Fuel using SCALE (No. ORNL/TM-2011/290, 1028163). <https://doi.org/10.2172/1028163>
- Alonso, C., Fernandez, L., 2004. Dehydration and rehydration processes of cement paste exposed to high temperature environments. *Journal of Materials Science* 39, 3015–3024. <https://doi.org/10.1023/B:JMSC.0000025827.65956.18>
- Andreani, M., Haller, K., Heitsch, M., Hemström, B., Karppinen, I., Macek, J., Schmid, J., Paillere, H., Toth, I., 2008. A benchmark exercise on the use of CFD codes for containment issues using best practice guidelines: A computational challenge. *Nuclear Engineering and Design* 238, 502–513. <https://doi.org/10.1016/j.nucengdes.2007.01.021>
- ANSYS, 2018. CFX-Solver Modeling Guide 688.
- Ashby, M.F., 2011. Designing Hybrid Materials, in: *Materials Selection in Mechanical Design*. Elsevier, pp. 299–340. <https://doi.org/10.1016/B978-1-85617-663-7.00011-4>
- ASM HANDBOOK VOLUME 1: Properties and Selection: Irons, Steels, and High-Performance Alloys, 1992. 2521.
- Baker, T.J., 2019. Fluent User's Guide 4088.
- Baldwin, B., Barth, T., 1991. A one-equation turbulence transport model for high Reynolds number wall-bounded flows, in: 29th Aerospace Sciences Meeting. Presented at the 29th Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics, Reno,NV,U.S.A. <https://doi.org/10.2514/6.1991-610>
- Barnhurst, R.J., Bean, J.C., Laboratories, T.B., Beaudry, B.J., Berry, D.F., Black, W.T., Bess, M., Biermann, R.J., Blackmon, C.M., Blaugher, R.D., 1992. ASM HANDBOOK: VOLUME " Properties and Selection: Nonferrous Alloys and Special-Purpose Materials 3470.
- Benavides, J., 2016. Análisis térmico del proceso de secado y almacenamiento de un contenedor de combustible nuclear gastado con CFD.
- Benavides, J., 2015. Evaluación térmica de un contenedor de combustible nuclear gastado con dinámica de fluidos computacional.
- Benavides, J., Jimenez, G., Galbán, M., Lloret, M., 2019. Methodology for thermal analysis of spent nuclear fuel dry cask using CFD codes. *Annals of Nuclear Energy* 133, 257–274. <https://doi.org/10.1016/j.anucene.2019.05.026>
- Benavides, J., Varas, G.J., Barahona, M.G., Llorca, M.L., Rusiñol, C.S., 2018. Estudio de los mecanismos de refrigeración del exterior del contenedor de combustible gastado TN-24P con STAR-CCM+. *Sociedad Nuclear Española* 8.
- BENCHMARKS FOR UNCERTAINTY ANALYSIS IN MODELLING (UAM) FOR THE DESIGN, OPERATION AND SAFETY ANALYSIS OF LWR, 2013.
- Boussinesq J, 1877. Essai sur la théorie des eaux courantes. *Mémoires présentés par divers savants à l'Académie des Sciences* 23.
- Brewster, R.A., Baglietto, E., Volpenhein, E., Bajwa, C.S., 2012a. CFD analyses of the TN-24P PWR spent fuel storage cask. *American Society of Mechanical Engineers, Pressure Vessels and Piping Division (Publication) PVP* 3. <https://doi.org/10.1115/PVP2012-78491>
- Cheng, X., Müller, U., 1998. Turbulent natural convection coupled with thermal radiation in large vertical channels with asymmetric heating. *International Journal of Heat*

- and Mass Transfer 41, 1681–1692. [https://doi.org/10.1016/S0017-9310\(97\)00303-7](https://doi.org/10.1016/S0017-9310(97)00303-7)
- Churchill, S.W., Chu, H.H.S., 1975. Correlating equations for laminar and turbulent free convection from a vertical plate. *International Journal of Heat and Mass Transfer* 18, 1323–1329. [https://doi.org/10.1016/0017-9310\(75\)90243-4](https://doi.org/10.1016/0017-9310(75)90243-4)
- CSN, 2013. Resolución por la que se aprueba la revisión 10 del Estudio Genérico de Seguridad del contenedor ENSA-DPT para el uso en una instalación de almacenamiento de combustible gastado.
- CSN, 2011. Ficha HI-STORM.
- Daly, B.J., Harlow, F.H., 1970. Transport Equations in Turbulence. *Phys. Fluids* 13, 2634. <https://doi.org/10.1063/1.1692845>
- Durbin, P.A., 1991a. Near-Wall Turbulence Closure Modeling Without “Damping Functions” 13.
- Durbin, S., Lindgren, E.R., 2017a. Thermal-Hydraulic Results for the Boiling Water Reactor Dry Cask Simulator. <https://doi.org/10.2172/1398335>
- ENSA, 2014. Entrada-DPT-30-en-ATI [WWW Document]. URL <https://www.ensa.es/cn-trillo-carga-de-contenedores-dpt-por-ensaenwesa/>
- EPRI, 1987a. The TN-24P PWR Spent-Fuel Storage Cask: Testing and Analyses.
- Equipos Nucleares, SA (ENSA), 2015. Aprobación del diseño del contenedor ENUN 32P para almacenamiento de combustible gastado en instalaciones de almacenamiento autorizadas.
- Eric W. Lemmon, Mark O. McLinden, Daniel G. Friend, 2019. Thermophysical Properties of Fluid Systems.
- Galbán, M., Lloret, M., Benavides, J., Jiménez, G., 2018. TEMPERATURE CALCULATIONS IN SPENT NUCLEAR FUEL CASK USING COBRA-SFS. TopFuel Prague September 2018 8.
- Greene, S.R., Medford, J.S., Macy, S.A., 2013. Storage and Transport Cask Data For Used Commercial Nuclear Fuel.
- Greene, S.R., Medford, J.S., Macy, S.A., n.d. Storage and Transport Cask Data For Used Commercial Nuclear Fuel.
- Hanson, B., Alsaed, H., Stockman, C., Enos, D., Meyer, R., Sorenson, K., 2012. Gap Analysis to Support Extended Storage of Used Nuclear Fuel Rev. 0.
- Harlow, F.H., 2004. Fluid dynamics in Group T-3 Los Alamos National Laboratory. *Journal of Computational Physics* 195, 414–433. <https://doi.org/10.1016/j.jcp.2003.09.031>
- Herranz, L.E., Penalva, J., Fera, F., 2015. CFD analysis of a cask for spent fuel dry storage: Model fundamentals and sensitivity studies. *Annals of Nuclear Energy* 76, 54–62. <https://doi.org/10.1016/j.anucene.2014.09.032>
- Hess, J.L., Smith, A.M.O., 1967. Calculation of potential flow about arbitrary bodies. *Progress in Aerospace Sciences* 8, 1–138. [https://doi.org/10.1016/0376-0421\(67\)90003-6](https://doi.org/10.1016/0376-0421(67)90003-6)
- Hunt, J.C.R., 1998a. LEWIS FRY RICHARDSON AND HIS CONTRIBUTIONS TO MATHEMATICS, METEOROLOGY, AND MODELS OF CONFLICT. *Annual Review of Fluid Mechanics* 30, xiii–xxxvi. <https://doi.org/10.1146/annurev.fluid.30.1.0>
- IAEA, 2018a. Status and Trends in Spent Fuel and Radioactive Waste Management.
- IAEA, 2018b. REGULATIONS FOR THE SAFE TRANSPORT OF RADIOACTIVE MATERIAL.
- Incropera, F.P., DeWitt, D.P., Bergman, T.L., Lavine, A.S. (Eds.), 2013. Principles of heat and mass transfer, 7. ed., international student version. ed. Wiley, Singapore.

-
- Jeong, Y.S., Bang, I.C., 2016. Hybrid heat pipe based passive cooling device for spent nuclear fuel dry storage cask. *Applied Thermal Engineering* 96, 277–285. <https://doi.org/10.1016/j.applthermaleng.2015.11.086>
- Johnson, F.T., Tinoco, E.N., Yu, N.J., 2005. Thirty years of development and application of CFD at Boeing Commercial Airplanes, Seattle. *Computers & Fluids* 34, 1115–1151. <https://doi.org/10.1016/j.compfluid.2004.06.005>
- Joint Convention on the Safety of Spent Fuel Management and on the Safety of Radioactive Waste Management: —Third Review Meeting of the Contracting Parties—, 2009. . *atomos* 51, 640–640. https://doi.org/10.3327/jaesjb.51.8_640
- Jones, W.P., Launder, B.E., 1972. The prediction of laminarization with a two-equation model of turbulence. *International Journal of Heat and Mass Transfer* 15, 301–314. [https://doi.org/10.1016/0017-9310\(72\)90076-2](https://doi.org/10.1016/0017-9310(72)90076-2)
- Kim, H.-G., Jeong, Y.-H., Kim, K.-T., 2010. THE EFFECTS OF CREEP AND HYDRIDE ON SPENT FUEL INTEGRITY DURING INTERIM DRY STORAGE. *Nuclear Engineering and Technology* 42, 249–258. <https://doi.org/10.5516/NET.2010.42.3.249>
- Kim, Y.-J., Kook, D.-H., Kim, T.-H., Kim, J.-S., 2015. Stress and temperature-dependent hydride reorientation of Zircaloy-4 cladding and its effect on the ductility degradation. *Journal of Nuclear Science and Technology* 52, 717–727. <https://doi.org/10.1080/00223131.2014.978829>
- Kolmogorov, A.N., 1991a. Dissipation of Energy in the Locally Isotropic Turbulence. *Proceedings: Mathematical and Physical Sciences* 434, 15–17.
- Kolmogorov, A.N., 1991b. The local structure of turbulence in incompressible viscous fluid for very large Reynolds numbers. *Proc. R. Soc. Lond. A* 434, 9–13. <https://doi.org/10.1098/rspa.1991.0075>
- Kumar, R., Dewan, A., 2016. A study of LES-SGS closure models applied to a square buoyant cavity. *International Journal of Heat and Mass Transfer* 98, 164–175. <https://doi.org/10.1016/j.ijheatmasstransfer.2016.02.057>
- Lee, J.C., Choi, W.S., Bang, K.S., Seo, K.S., Yoo, S.Y., 2009. Thermal-fluid flow analysis and demonstration test of a spent fuel storage system. *Nuclear Engineering and Design* 239, 551–558. <https://doi.org/10.1016/j.nucengdes.2008.12.015>
- Lien, F.S., Chen, W.L., Leschziner, M.A., 1996a. Low-Reynolds-Number Eddy-Viscosity Modelling Based on Non-Linear Stress-Strain/Vorticity Relations, in: *Engineering Turbulence Modelling and Experiments*. Elsevier, pp. 91–100. <https://doi.org/10.1016/B978-0-444-82463-9.50015-0>
- Lien, F.S., Kalitzin, G., Durbin, P.A., 1998. RANS modeling for compressible and transitional flows 20.
- Lindgren, E.R., Durbin, S., 2017a. Materials and Dimensional Reference Handbook for the Boiling Water Reactor Dry Cask Simulator. (No. SAND2017- 13058R, 1559567). <https://doi.org/10.2172/1559567>
- Martínez, C.B., 2002. Resolución de la Dirección General de Política Energética y Minas por la que se aprueba el contenedor ENSA-DPT para uso en instalaciones de almacenamiento de combustible irradiado&MISTERIO DE ECONOMIA. Ministerio de Economía 7.
- McAdams, William H., 1954a. *Heat Transmission* (3d ed).
- Mikulčić, H., Vujanović, M., Fidaros, D.K., Priesching, P., Minić, I., Tatschl, R., Duić, N., Stefanović, G., 2012. The application of CFD modelling to support the reduction of CO₂ emissions in cement industry. *Energy* 45, 464–473. <https://doi.org/10.1016/j.energy.2012.04.030>

- Montefuel, R.D., 1993. Heat transfer in Enclosed Rod Array.
- Montefuel, R.D., Neil, E.T., 1993. Effective Thermal conductivity and edge conductance model for a spent fuel assembly.
- Moukalled, F., Mangani, L., Darwish, M., 2016. The Finite Volume Method in Computational Fluid Dynamics: An Advanced Introduction with OpenFOAM® and Matlab, Fluid Mechanics and Its Applications. Springer International Publishing, Cham. <https://doi.org/10.1007/978-3-319-16874-6>
- Nagano, Y., Abe, K., Kondoh, T., 1994a. A new turbulence model for predicting fluid flow and heat transfer in separating and reattaching flows-I. Flow field calculations K.ABE and T. KONDOCH Toyota Central Research and Development laboratories, Inc., Nagakute~ho, Aichi-ken 480-I I, Japan Aichi-gun, 13.
- Norton, T., Sun, D.-W., 2006. Computational fluid dynamics (CFD) – an effective and efficient design and analysis tool for the food industry: A review. Trends in Food Science & Technology 17, 600–620. <https://doi.org/10.1016/j.tifs.2006.05.004>
- Orano-MP197HB-shielded-transport-cask [WWW Document], 2021. . World Nuclear News. URL <https://www.world-nuclear-news.org/Articles/New-transport-cask-is-ready-for-first-US-deploymen>
- Pacific Northwest Laboratory, 2018a. COBRA-SFS CYCLE 4A:Code System for Thermal Hydraulic Analysis of Spent Fuel Casks.
- Patankar, S.V, Spalding, D.B, 1971. A calculation procedure for heat, mass and momentum transfer in three-dimensional parabolic flows. International Journal of Heat and Mass Transfer 15, 1787–1806.
- Posiva Oy, 2020. ONKALO in landscape [WWW Document].
- Prandtl, L, 1949. Translation of “ Bericht fiber Untersuchungen zur ausgebildeten Turbulent.” Zeitschrift fiir angewand~e Mathematik und Mechanik, vol. 5, no. 2, April 1925.
- Pulido, R.J.M., Lindgren, E.R., Durbin, S.G., Zigh, A., Solis, J., Suffield, S.R., Richmond, D.J., Fort, J.A., Herranz, L.E., Feria, F., Penalva, J., Lloret, M., Galbán, M., Benavides, J., Jiménez, G., 2019a. Spent Fuel and Waste Disposition 72.
- Remache, A., Addad, Y., Sabeur-Bendehina, A., Ouadha, A., 2019. Thermal design optimization of passive cooling capability in a dry-storage system by adding wall undulations or semi-circular fins. Nuclear Engineering and Design 347, 140–150. <https://doi.org/10.1016/j.nucengdes.2019.03.028>
- Rieutord, M., 2015. Fluid Dynamics, Graduate Texts in Physics. Springer International Publishing, Cham. <https://doi.org/10.1007/978-3-319-09351-2>
- Roache, P.J., 1994. Perspective: A Method for Uniform Reporting of Grid Refinement Studies. Journal of Fluids Engineering 116, 405. <https://doi.org/10.1115/1.2910291>
- Rodi, W., 1991. Experience with two-layer models combining the k-epsilon model with a one-equation model near the wall, in: 29th Aerospace Sciences Meeting. Presented at the 29th Aerospace Sciences Meeting, American Institute of Aeronautics and Astronautics, Reno,NV,U.S.A. <https://doi.org/10.2514/6.1991-216>
- Rosa, M.D., Guetta, G., Ambrosini, W., Forgiione, N., He, S., Jackson, J.D., 2011. LESSONS LEARNED FROM THE APPLICATION OF CFD MODELS IN THE PREDICTION OF HEAT TRANSFER TO FLUIDS AT SUPERCRITICAL PRESSURE 13.

-
- SEPI, 2019. ENSA envía su segundo contenedor ENUN 32P a la central nuclear de Almaraz [WWW Document]. URL <http://www.sepi.es/es/sala-de-prensa/noticias/ensa-envia-su-segundo-contenedor-enun-32p-la-central-nuclear-de-almaraz> (accessed 7.16.20).
- Serrano, J., 2001. Caracterización y lixiviación de combustibles nucleares irradiados y de sus análogos químicos,. Madrid.
- SIEMENS, 2018a. STAR-CCM+ 13.02 USER GUIDE.
- Singh, R.N., Kishore, R., Sinha, T.K., 2002. Studies on Stress reorientation of hydrides in Zr-2.5Nb pressure tube alloy.
- Sorenson, K., Kessler, J., 2012. International Perspectives on Technical Data Gaps Associated with Long Term Storage and Transportation of Used Nuclear Fuel Ken Sorenson.
- Tipos de contenedores - CSN [WWW Document], 2008. URL <https://www.csn.es/contenedores-de-almacenamiento-de-combustible-gastado/tipos-de-contenedores> (accessed 6.23.20).
- US NRC, 2020a. PWR Fuel assembly [WWW Document]. URL <https://www.nrc.gov/reading-rm/basic-ref/students/for-educators/reactor-fuel-assembly.html>
- US NRC, 2020b. Exterior temporal storage site [WWW Document]. URL https://en.wikipedia.org/wiki/Dry_cask_storage#/media/File:Nuclear_dry_storage.jpg
- USNRC, 2012. Characterization of Thermal-Hydraulic and Ignition Phenomena in Prototypic, Full-Length Boiling Water Reactor Spent Fuel Pool Assemblies After a Postulated Complete Loss-of-Coolant Accident Office.
- U.S.NRC, 2010. Standard Review Plan for Spent Fuel Dry Storage Systems at a General License Facility Final Report 1–424.
- USNRC, 2003. Spent Fuel Project Office, Interim Staff Guidance N° 11, Revision 3.
- Wolfstein, M., 1969a. The velocity and temperature distribution in one-dimensional flow with turbulence augmentation and pressure gradient.
- Xu, W., Chen, Q., Nieuwstadt, F.T.M., 1998a. A new turbulence model for near-wall natural convection. *International Journal of Heat and Mass Transfer* 41, 3161–3176. [https://doi.org/10.1016/S0017-9310\(98\)00081-7](https://doi.org/10.1016/S0017-9310(98)00081-7)
- Yoo, H.S., Yoo, S.H., Kim, E.S., 2019. Heat transfer enhancement in dry cask storage for nuclear spent fuel using additive high density inert gas. *Annals of Nuclear Energy* 132, 108–118. <https://doi.org/10.1016/j.anucene.2019.04.018>
- Yoo, S.H., No, H.C., Kim, H.M., Lee, E.H., 2010a. Full-scope simulation of a dry storage cask using computational fluid dynamics. *Nuclear Engineering and Design* 240, 4111–4122. <https://doi.org/10.1016/j.nucengdes.2010.08.009>
- Yoo, S.H., No, H.C., Kim, H.M., Lee, E.H., 2010b. CFD-assisted scaling methodology and thermal-hydraulic experiment for a single spent fuel assembly. *Nuclear Engineering and Design* 240, 4008–4020. <https://doi.org/10.1016/j.nucengdes.2010.03.004>
- Zhang, Z., Zhang, W., Zhai, Z.J., Chen, Q.Y., 2007. Evaluation of various turbulence models in predicting airflow and turbulence in enclosed environments by CFD: Part 2—comparison with experimental data from literature. *HVAC and R Research* 13, 871–886. <https://doi.org/10.1080/10789669.2007.10391460>
- Zhang, Z., Zhang, W., Zhai, Z.J., Chen, Q.Y., Zhai, Z.J., Chen, Q.Y., 2011. Evaluation of Various Turbulence Models in Predicting Airflow and Turbulence in Enclosed Environments by CFD : Part 2 — Comparison with Experimental Data from

Literature Evaluation of Various Turbulence Models in Predicting Airflow and Turbulence in Enclo 9669. <https://doi.org/10.1080/10789669.2007.10391460>
Zigh, C., Solis, J., 2013. Computational Fluid Dynamics Best Practice Guidelines for Dry Cask Applications Final Report.