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Sub-Channel CFD for Nuclear Fuel Bundles

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Abstract

This paper presents a novel Computational Fluid Dynamics (CFD)-based sub-channel framework for nuclear power plants, which combines the advantageous features of modern CFD and traditional 1-D sub-channel codes. The new method is capable of producing CFD-level 3-D results with locally desirable refinement when coupled with embedded resolved models, but because a very coarse mesh is used over most part of the domain, the computing cost is typically significantly smaller than that of a conventional CFD simulation.

In this new Sub-Channel CFD (SubChCFD), a dual-mesh system is used, comprising, (i) a filtering mesh which aligns with the mesh used in typical sub-channel codes, enabling the use of existing engineering correlations to account for integral wall friction and heat transfer effects, and (ii) a computing mesh, which provides a platform for the solution of the governing equations with turbulence modelled using a mixing-length-type model. The method has been implemented in an open-source finite volume CFD code Code_Saturne and validated initially using a 5×5 bare bundle case based on the OECD/NEA MATiS-H benchmarking experiment. It has been found that SubChCFD is able of satisfactorily predicting both the velocity and temperature fields. To further investigate the performance for complex flow conditions, SubChCFD was applied to two full 3-D cases. The first is a 5×5 rod bundle case with local blockage in one of the sub-channels, creating significant localised cross flows. The second is a two-parallel-assembly channel with different input mass flow rates at the inlet of each assembly, allowing strong inter-assembly mixing. For both cases, SubChCFD has produced results which agree well with experiments and simulations using resolved CFD. It has also been demonstrated that SubChCFD exhibits excellent flexibility in comparison with traditional sub-channel codes and that it has the potential to serve as a substitution to sub-channel codes.

Keywords

Nuclear reactor, CFD, Heat transfer, Sub-Channel, Coarse-Grid

1. Introduction

To leverage the aggravation of the global environmental crisis, such as global warming and climate change, arising from the consumption of carbon-based fuel, nuclear power will continue to play an important role in energy generation due to its low emission of greenhouse gases. There are currently about 440 nuclear power plants in operation around the world and over 120 new reactors under construction (Moorthi et al., 2018). Following lessons learned from some major nuclear accidents, especially the most important one in Fukushima in 2011, passive cooling and margin management have proven to be increasingly prominent. In addition to steady-state normal operating conditions, safety assessment of the modern nuclear system needs to consider a variety of additional scenarios, such as: operational transients (e.g. start-up, and shut-down); anticipated off-design operation (for activities such as refuelling) and a wide variety of postulated fault and accident conditions, to enable fault recovering strategies to be developed and also to minimise the risk of radiological release.

The safety assessment of a nuclear reactor core and its associated components strongly relies on thermal hydraulic analysis of the coolant by means of experimental investigation or numerical simulations (Sha, 1980; Yadigaroglu et al., 2003). Restricted by the computational power in the 1960s to 1980s, the thermal hydraulic calculations were mainly performed using the best-estimate system codes such as RELAP5 (RELAP5 Development Team, 1995), ATHLET (Lerchl et al., 2012), CATHARE (Bestion, 1990) and TRAC (Liles and Mahaffy, 1986), and sub-channel codes such as COBRA (Rowe, 1967), VIPRE (Stewart et al., 1983) and MATRA (Hwang et al., 2008).The former are usually used to analyse the overall behaviour of the whole system under different operating conditions, whereas the latter provide a relatively detailed thermal hydraulic analysis at the fuel channel level by solving 1-D transport equations based on individual flow passages formed between fuel rods or fuel rods and walls, i.e. the so-called sub-channels. These transport equations are based on empirical correlations to account for un-resolved physics, such as frictional loss, spacer induced effects, turbulence, inter-channel mixing, and void drifting, etc. As such, sub-channel analysis codes are able to provide numerical predictions at a resolution of the sub-channel scale, which was state-of-the-art in 1-D approaches at that time. However, it is more and more likely that traditional 1-D codes are no longer sufficient in meeting the requirements of modern reactor design and safety case development (Brockmeyer et al., 2016; Jeong et al., 2005), despite the fact that they are able to provide an answer quickly. The rapid increase in computational power in the last several decades allows the advanced Computational Fluid Dynamics (CFD) methods to be used by reactor developers to study some complex 3-D physics of coolant flow in nuclear fuel channels. This has the potential to significantly re-shape future nuclear thermal hydraulic analysis.

63 Due to the complex internal structure, the scales of the flow in a nuclear reactor span a large range, varying

64 from sub-millimeter (e.g. secondary flow in fuel assemblies) to meters or even tens of meters (e.g. natural

65 circulation in a loss of coolant accident (LOCA)) (Yu et al., 2017). This requires the computational

66 domain of a CFD model to be meshed using a fine grid to allow most physical scales to be captured.

67 Consequently, it is still not practical to carry out core-level CFD simulations due to the prohibitive

68 computing expense even with today's high-performance computing systems. Alternatively, CFD

69 simulations can be carried out for representative sections with properly defined boundary conditions to

70 reduce the computing cost by taking advantage of the fact that the core structures are typically spatially

71 periodic in a nuclear reactor. Such an approach has been used by various researchers to carry out CFD

72 analysis for single channels (Cui and Kim, 2003; Házi, 2005; Imaizumi et al., 1995; Karouta et al., 1995),

73 multiple channels (G. Chen et al., 2017; Han et al., 2017; Liu et al., 2012; Liu and Ferng, 2010; Tseng et

74 al., 2014; Zhao et al., 2017), rod bundle arrays (Agbodemegbe et al., 2016; Ala et al., 2017; Bieder, 2017;

75 Bieder et al., 2014; Denefle et al., 2017; Ikeda, 2014; Kang and Hassan, 2016), reactor core sectors

76 (Simoneau et al., 2007; Takamatsu, 2017; Tsuji et al., 2014), and plena (M. Kao et al., 2010; Kao et al.,

77 2011), etc. With the experiences accumulated in academia, CFD is further used in industry to optimise

78 the design of some key components of reactors, such as spacer grids of a Pressurised water reactor (PWR)

79 fuel assembly (Ikeda, 2014; Podila et al., 2013). Among these studies and applications, the wall-function

80 Reynolds averaged Navier-Stokes (RANS) methods, especially the k- ε series models were often used in

81 early research (Cui and Kim, 2003; Házi, 2005; Imaizumi et al., 1995) or the modelling of large

82 components (M. Kao et al., 2010; Kao et al., 2011; Simoneau et al., 2007; Takamatsu, 2017; Tsuji et al.,

83 2014) as they can provide reasonable predictions at relatively small costs since the near-wall region is not

84 resolved. However, the methods are no longer satisfactory for cases with complex flow phenomena, such

85 as adverse pressure gradient, vortex shedding, impingement, swirling, and buoyancy influenced flows,

86 etc. In such cases, more sophisticated methods are usually required for better predictions, such as

87 anisotropic Reynolds-Stress Models (RSM) and low Reynolds number RANS or unsteady RANS models

88 (X. Chen et al., 2017; M.-T. Kao et al., 2010) in which the boundary layer can be resolved down to the

89 viscous sub-layer using high-resolution near-wall meshes with the first cell y+ up to 1.0. In addition, the

90 state-of-the-art high-fidelity methods, e.g. Large Eddy Simulation (LES) and Direct Numerical

91 Simulation (DNS) have also been used by many researchers in nuclear thermal hydraulics

92 (Benhanmadouche et al., 2009; Fischer et al., 2007; Shams et al., 2013). Due to the extremely high cost

93 of the latter methods, they cannot be widely used in engineering, especially DNS which is still restricted

94 to simple geometries and low Reynolds numbers. However, they are normally used to generate

95 benchmarking dataset for the development of new RANS turbulence models or as numerical tools for the

96 fundamental study of turbulence.

97 Work has been done to make use of the advancement of modern CFD in core-level or even system-level

98 modelling by coupling it with low cost simpler methods. In such approaches, CFD usually takes the role

99 of capturing the complex 3-D flow of the most interesting regions/sections in the reactor system, whilst

100 the rest is described using simplified models. The information exchange between the different models is

101 challenging, which can be explicit or implicit in time and spatially decomposed or overlapped, depending

102 on the method used (Grunloh and Manera, 2016).

103 At system level, CFD can be coupled to system codes to enhance their performance in predicting the

104 complex behaviour of the entire nuclear power plant (NPP) under non-design conditions. To date,

105 tremendous efforts have been dedicated to enabling the coupling between CFD and system codes.

106 Anderson et al. (2008) analysed a very high-temperature reactor (VHTR) using a coupled RELAP/CFD

107 system where the 3-D flow in the outlet plenum was modelled using CFD. Papukchiev et al. (2011)

108 coupled ATHLET and ANSYS CFX, and then validations were done based on a pressure thermal shock

109 related experiment for pressurized water-cooled reactor (PWR). Bury (2013) studied a reactor

110 containment system under a scenario of LOCA using an in-house system code HEPCAL-AD coupled

111 with ANSYS FLUENT. The natural circulation within an annular channel between an inner steel vessel

112 and the containment wall was simulated using CFD. Bavière et al. (2014) simulated a sodium-cooled

113 nuclear system with a coupled simulation of CATHARE2 and Trio_U, which allows energy and

114 momentum feedback from CFD to the system code. Toti et al. (2017) implemented an implicit domain

115 decomposition algorithm to enable the coupling between the system code RELAP5-3D and ANSYS

116 FLUENT for high fidelity safety analyses of pool-type reactors. The method showed good agreement with

117 the experimental data of a loss of flow transient induced by local 3-D phenomena. Despite the encouraging

118 progress, there are two challenges in such code couplings. One is the low convergence rate due to the

119 weak coupling, e.g. using a time explicit scheme in which the information is only exchanged once at the

120 end of each time step. The other major challenge is that it is difficult to develop a generic library that can

121 be used for different pairs of coupling codes, because of their very different data structures.

122 At core-level, one of the most popular approaches used in the open literature is to couple the porous media

123 model with the well-resolved CFD to reduce the computing cost. In some of the cases, porous media is

124 used to describe fuel assemblies (Chen et al., 2015; Fiorina et al., 2015; Skibin et al., 2017; Yu et al.,

125 2015), others also include plena (Brewster et al., 2017; R. Chen et al., 2017). Some researchers have

126 developed alternative ways to simplify the core modelling. For example, Corzo et al. (2015) incorporated

127 a 1-D finite volume code to account for the complex fuel channels in a full core simulation of a pressurised

128 heavy water reactor. Zhang et al. (2013) employed a distributed resistance model to represent the core

129 module of a real geometry model of a PWR, whilst a detailed model was used for the down-comer and

130   the lower plenum. These simplified methods are, to some extent, similar to sub-channel codes, in which

131   either the flow is forced in a single direction, or the geometry of the fuel rods is not taken into account

132   explicitly. As such, these approaches are not suitable to capture small to medium scaled 3-D transient

133   features, for example, the recirculation behind a blockage.

134   A new interesting area of research is the development of unresolved, coarse grid CFD to enable relatively

135   large flow systems to be simulated at a low cost. Along this line of research, Hu and Fanning (2013)

136   introduced a 3-D momentum source term method to simulate anisotropic flows in fuel channels of wire-

137   wrapped bundles without fully resolving the geometrical details of the wires with fine meshes. Bieder et

138   al. (2010) also studied wire-wrapped bundles using a low-resolution method, but differing from Hu and

139   Fanning. They simplified the mesh generation by replacing the wire wrap with a spinal fin. Roelofs et al.

140   (2012) proposed a method referred to as Low-Resolution Geometry Resolving (LRGR) CFD which

141   captures 'medium scale' flow features without a sub-grid model in the case that secondary flows are not

142   important. Class et al. (2011) and Viellieber and Class (2012) employed an even coarser mesh in their

143   approach, referred to as Coarse-Grid CFD (CG-CFD), to make the simulation as efficient as sub-channel

144   codes but without depending on experimental data. They solve the Euler equations instead of the Navier-

145   Stokes equations with diffusion effects accounted for using a volumetric force extracted from detailed

146   simulations pre-performed on the same geometry. This approach has to date not been applied to heat

147   transfer where the parametric procedure could be a challenge due to the coupling between momentum and

148   energy transport. Along a totally new line, Hanna et al. (2017) associated the local error arising from grid

149   coarsening to features of the mesh by training a surrogate statistical model with detailed simulation results

150   using the state-of-the-art machine learning technology and then tested their method on a 3D lid-driven

151   cavity flow.

152   In conclusion, although great advances have been made in CFD over the past few decades, which enable

153   many problems previously only tackled by experiments to be solved by means of numerical simulation

154   (thus saving considerable resources), the application of CFD in real-life engineering is still limited by its

155   high computing cost. Additionally, CFD is a generic tool which is not developed specifically for nuclear

156   applications. The uncertainties related to numerical strategies, user inputs (e.g., initial and boundary

157   conditions), and turbulence models are very difficult to measure and control due to the generality,

158   complexity and flexibility of the method. For these reasons, reactor design and safety assessment in the

159   nuclear industry still largely rely on system and sub-channel codes.

160   To make use of the modelling techniques achieved in the booming development of CFD in nuclear

161   thermal-hydraulic modelling to supplement or potentially replace the lower-order methods, an effective

162   solution may be to implement some key concepts of the 1-D methods in the framework of modern CFD.

163 In doing so, the traditional 1-D tools could be modernised to have some CFD-like features with improved
164 flexibility, while maintaining the strengths of the system/sub-channel codes so as to provide performance
165 and accuracy that are at least as good as the system/sub-channel codes without a significant increase in
166 computing cost. Thanks to the use of the CFD platform, this approach will have the potential to be easily
167 coupled with traditional CFD methods, thus circumventing a series of difficulties and problems
168 encountered in coupling between different platforms.

169 The purpose of this paper is to present a novel coarse grid CFD technique following the aforementioned
170 approach. Unlike the methodology of other coarse grid CFD, e.g., Class et al. (2011), Viellieber and Class,
171 (2012) and Hanna et al. (2017), which is aimed at alleviating the dependence on experiments and
172 empiricism, our method can best be described as a low-resolution CFD using a correlation-based model
173 closure method, in which the experimental and engineering data are used whenever possible. In this
174 method, the inviscid flow with corrections for mixing is solved on a very coarse grid using a standard
175 CFD solver while the empirical correlations of the frictional loss and heat transfer are used to ensure
176 correct integral effects of the solid walls.

177 Section 2 introduces the methodology of the novel coarse grid CFD, Section 3 presents its validation and
178 application to several test cases and Section 4 provides some recommendations.

2. Methodology

180 The novel method presented herein is a new coarse grid CFD solver coupled with an embedded sub-
181 channel model, which is referred to as sub-channel CFD or SubChCFD. The method adopts a dual
182 mesh/dual solution methodology, namely, (i) a filtering mesh which aligns with the mesh used in typical
183 sub-channel codes, enabling the integral wall friction and heat transfer effects calculated using existing
184 engineering correlations, and (ii) a computing mesh, on which the RANS equations with a simple mixing
185 length-type model are solved. The former is also referred to as the sub-channel mesh/calculation and the
186 latter to the CFD mesh/solution. The friction and heat transfer calculated from the sub-channel solution
187 are used in the CFD via boundary conditions to ensure that the integral effect of the flow solution is
188 consistent with existing engineering correlations. On the other hand, the detailed CFD results are
189 integrated over the sub-channel cells to produce the integral flow parameters (e.g. velocity, thermal
190 properties), which are used in the sub-channel calculations.

191 The mapping between the filtering mesh and the computing mesh is established through geometrical
192 relations so that any physical parameters and field variables stored on the latter can be used directly to
193 produce corresponding sub-channel quantities for the former by spatial averaging, i.e.

$$\varphi_{sub,j} = \sum_{i \in j} \left(\frac{V_i}{V_{sub,j}} \right) \varphi_i \qquad (1)$$

194

195   where $\varphi_{sub,j}$ is the sub-channel-level quantity of φ on the jth filtering mesh element, φ_i the CFD-level

196   quantity of φ on the ith computing mesh element, V_i the volume of the ith computing mesh element, $V_{sub,j}$

197   the volume of the jth filtering mesh element.

198   With the advancement of the iteration process, information is continually exchanged between the

199   computing mesh and the filtering mesh, and finally, the CFD solution obtained and the empirical

200   correlations at the sub-channel level are consistent with each other. In practice, this can be achieved when

201   the CFD solver reaches convergence on the computing mesh, because the correlations are used as

202   boundary conditions in the CFD simulation. The detailed procedure of the algorithm of SubChCFD is

203   presented in Figure 1.
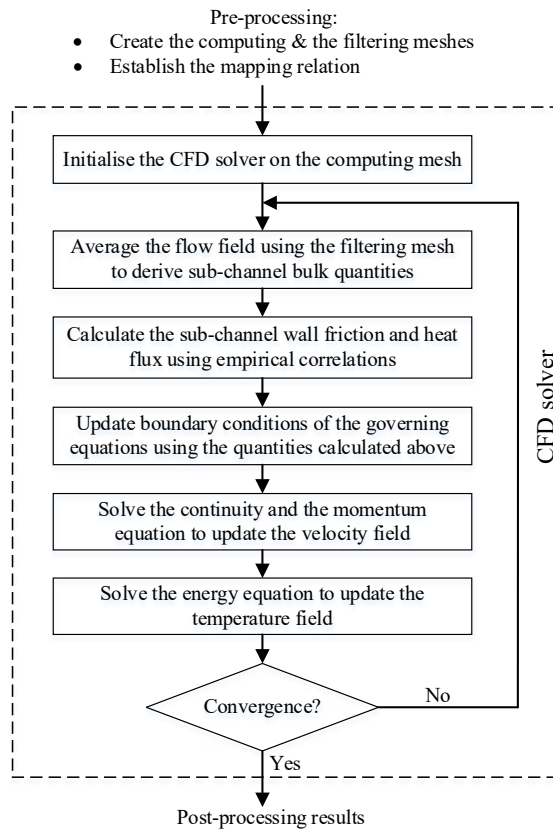
204

205   **Fig. 1 Details of the SubChCFD methodology**

206   The RANS governing equation to be solved in SubChCFD can be expressed as

207
$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \rho \vec{u} \otimes \vec{u} = -\nabla p + \nabla \cdot \overline{\sigma} + \vec{S}_u \tag{2}$$

208 where $\overline{\sigma}$ is the stress tensor including both the viscous and the turbulence contributions, $\vec{S}_u$ is the body

209 force. The discrete form is derived by integrating Equation (2) over each computing mesh cell Ω to yield:

210
$$\iiint_{\Omega} \frac{\partial \rho \vec{u}}{\partial t} dV + \oiint_{S} \vec{u}\left(\rho \vec{u} \cdot \vec{n}\right) dA = -\oiint_{S} \left(\overline{I}p \cdot \vec{n}\right) dA + \oiint_{S} \overline{\sigma} \cdot \vec{n} dA + \iiint_{\Omega} \vec{S}_u dV$$
$$= -\oiint_{S} \left(\overline{I}p \cdot \vec{n}\right) dA + \iint_{S_w} \overline{\sigma} \cdot \vec{n} dA + \iint_{S_f} \overline{\sigma} \cdot \vec{n} dA + \iiint_{\Omega} \vec{S}_u dV \tag{3}$$

211 where $S = S_w \bigcup S_f$, S_w is the cell surfaces adjacent to a wall boundary, S_f is the interior cell surfaces. The

212 convection term is discretised directly, whereas the viscous term requires some special care. During the

213 Stokes integration, the viscous term is decomposed into two parts which include the wall boundaries and

214 the interior interfaces, describing viscous forces between the wall and the adjacent fluid element and

215 viscous forces between fluid elements, respectively. Figure 2 shows an example of the mesh system used

216 for a PWR fuel channel where the physical meaning of the two parts of the viscous term is also clearly

217 demonstrated.
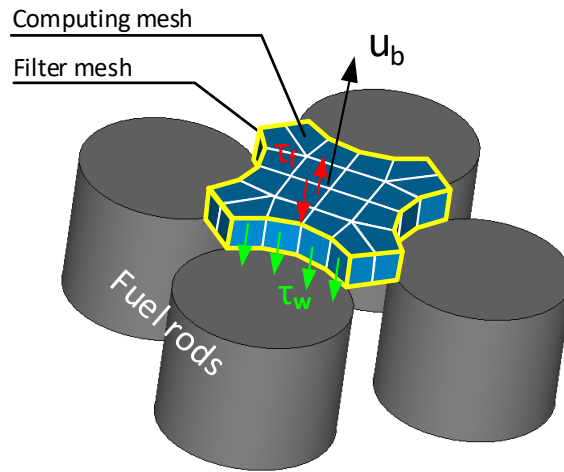
218
219 **Fig. 2 Mesh system in SubChCFD**

220 Since the mesh used in SubChCFD is very coarse, all the control volumes in the computational domain

221 can be safely assumed to be located in the core flow region sufficiently away from the wall effect.

222 Therefore, the discretisation of the interior part of the diffusion term, i.e. the second last term in Equation

223 (3), is not expected to have significant errors thanks to the relatively low velocity gradients occurring

224 there. The eddy viscosity is modelled using a simple model such as a 0-equation mixing length turbulence
225 model, which is used in this study. As such, the interior part can be finally written in the following form
226 and discretised.

227
$$\iint_{S_f} \bar{\sigma} \cdot \vec{n} dA = \iint_{S_f} (\mu + \mu_t) \left(\nabla \vec{u} + \nabla \vec{u}^T - \frac{2}{3} \delta \nabla \cdot \vec{u} \right) \cdot \vec{n} dA$$
(4)

228 where $\mu_t = \rho l_m^2 \sqrt{2 S_{ij} S_{ij}}$, the mixing length l_m can be calculated through $l_m = 0.09\Delta$ (Δ is the thickness of
229 the boundary layer, which takes a value of half the hydraulic diameter in bundle flows).

230 The wall-boundary part of the diffusion term, i.e. the third last term of Equation (3), can be calculated as
231 follows,

232
$$\iint_{S_W} \bar{\sigma} \cdot \vec{n} dA = \frac{1}{4} f \frac{1}{2} \rho_b \vec{u}_b |\vec{u}_b| \iint_{S_W} dA$$
(5)

233 where f denotes the skin fractional factor; ρ_b and $\vec{u}_b$ represent the sub-channel bulk density and bulk
234 velocity, respectively.

235 The energy equation,

236
$$C_p \left(\frac{\partial \rho T}{\partial t} + \nabla \cdot \rho \vec{u} T \right) = -\nabla \cdot \vec{q} + S_E$$
(6)

237 is treated in a similar way to generate an integrated form. It reads

238
$$C_p \left(\iiint_\Omega \frac{\partial \rho T}{\partial t} dV + \oiint_S \vec{u} (\rho T \cdot \vec{n}) dA \right) = -\oiint_S \vec{q} \cdot \vec{n} dA + \iiint_\Omega S_E dV$$
$$= -\iint_{S_W} \vec{q} \cdot \vec{n} dA - \iint_{S_f} \vec{q} \cdot \vec{n} dA + \iiint_\Omega S_E dV$$
(7)

239 The diffusion term of the energy equation is also split into a wall-boundary part and an interior part. The
240 interior part is calculated using

241
$$\iint_{S_f} \vec{q} \cdot \vec{n} dA = -\iint_{S_f} (\lambda + \lambda_t) \nabla T \cdot \vec{n} dA .$$
(8)

242 The diffusion term in the energy equation at the wall boundaries is determined using the sub-channel-
243 based Nusselt number correlations. The calculation of the wall-boundary part depends on the types of the
244 boundary condition of the solid walls. Table 1 shows the details of the calculation method for three
245 different types of thermal boundary conditions. It can be noted that, for the Dirichlet and Robin boundary
246 conditions, the Nusselt number is present in the calculation of the wall heat flux in the main solution loop
247 for the governing equations. As depending on the flow at the sub-channel level, the Nusselt number can
248 only be calculated using the information from the previous time step, that is, an explicit coupling between
249 the sub-channel and CFD solutions. Here, the sub-channel bulk temperature T_b is calculated using the
250 following equation,

251
$$T_b = \iiint_{\Omega_{sub}} \rho u T^{n-1} dV \Big/ \iiint_{\Omega_{sub}} \rho u dV$$
(9)

252 where T^{n-1} is the temperature at the previous time step, Ω_{sub} represents a cell of the filtering mesh.

253 The situation is much simpler for the case of the Neumann boundary condition as the wall heat flux is
254 given. The Nusselt number is only required for estimating the surface temperature of the walls during the
255 post-processing stage.

256 **Table 1 Near-wall part of the diffusion term in the energy equation**

Boundary types	Conditions	$\iint_{S_w} \vec{q} \cdot \vec{n} dA$
Dirichlet	$T\big|_{S_w} = T_w$	$-\dfrac{\lambda \mathrm{Nu}}{D_h}(T_w - T_b) \iint_{S_w} dA$
Neumann	$\dfrac{\partial T}{\partial n}\Big|_{S_w} = -q$	$q \iint_{S_w} dA$
Robin	$\left(aT + b\dfrac{\partial T}{\partial n}\right)\Big|_{S_w} = c$	$\dfrac{\lambda \mathrm{Nu}(aT_b - c)}{aD_h + b\mathrm{Nu}} \iint_{S_w} dA$

257

258 Due to the use of the coarse grid, SubChCFD is not expected to achieve complete mesh-independence of
259 the solution even though as it will be shown later in this Section 3.1.2, SubChCFD has demonstrated
260 rather small mesh-dependence. To further limit mesh-dependence, improve consistency in model

261 generation for different flow problems and improve the accuracy of the simulation, we note the following
262 guidelines on mesh generation:

1. The filtering mesh should be chosen closely following the sub-channel divisions used in
    traditional sub-channel codes where possible.
2. The computing mesh should be generated from the filtering mesh, effectively sub-dividing it into
    smaller cells.
3. Each sub-channel is divided into two regions, namely, the wall region and the core region.
4. Taking square-lattice PWR sub-channel as an example, we suggest three 'standard' mesh
    strategies for a 2-D cross section mesh of the sub-channels as outlined below (see Figure 3). They
    can be used directly to build the full 3-D mesh by axial extrusion.
    a) Mesh 1: The wall region is represented by a single wall-layer, comprising 4×1 cells; and
        the core is meshed by a 2×2 mesh.
    b) Mesh 2: The wall region is represented by two wall layers, comprising 6×2 cells; and the
        core is meshed by a 2×2 mesh.
    c) Mesh 3: The wall region is represented by two wall layers, comprising 8×2 cells; the core
        is meshed by a 4×4 mesh.

(a) Mesh-1   (b) Mesh-2   (c) Mesh-3   (d) CFD mesh
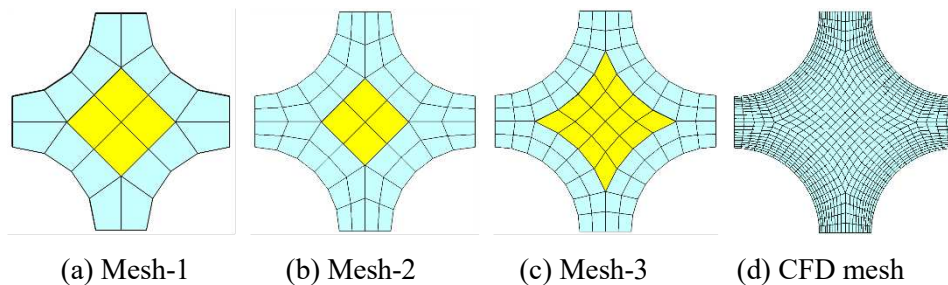
Fig. 3 Comparison of the computing mesh set in SubChCFD and a RANS wall-modelled CFD mesh for a square-lattice PWR sub-channel

281 The aforementioned mesh strategies allows SubChCFD to have a higher flexibility than the traditional 1-
282 D tools in capturing flow physics. It is expected that the users of SubChCFD will select a suitable strategy
283 for their purpose to balance resolution requirements and computing cost and will maintain the same mesh
284 for their application. In practice, the model parameters used in SubChCFD will be pre-calibrated taking
285 into account the mesh strategies to ensure an optimal performance when used for a specific type of nuclear
286 reactor. Figure 3 gives an example of the computing mesh set generated in line with the above mesh
287 strategies (see Mesh-1, Mesh-2, Mesh-3 on Figure 3 a, b and c, respectively) and a wall-modelled CFD
288 mesh for a square-lattice PWR sub-channel (see Figure 3 d). It can be seen clearly that the cell count in

289 SubChCFD is much smaller than that in the conventional CFD (in this case, 20, 52 and 80 cells in Mesh
290 1, 2 and 3, while 624 cells in the CFD mesh). Accordingly, the computing cost is expected to be reduced
291 by about 1 to 2 orders of magnitude in a 2-D case and 2 to 3 orders of magnitude in a full 3-D case,
292 respectively. This is just a comparison with the wall-modelled CFD, and the reduction in computing cost
293 will be even more significant when compared with wall-resolved CFD simulations.

3. Validation and Application

295 In this study, the multi-purpose CFD package Code_Saturne developed by EDF R&D (Fournier et al.,
296 2011) is used as the platform to implement SubChCFD. Code_Saturne is a finite-volume method based
297 open-source software, providing the user full access to the source code. A well-defined user subroutine
298 system allows the user to implement self-defined models and methods easily and conveniently.

3.1 Fully developed flow and heat transfer in a 5×5 PWR bundle

3.1.1 Description of the test case

301 To demonstrate and validate the new methodology of SubChCFD in nuclear thermal-hydraulic modelling,
302 a 2-D model is firstly created to simulate an axially fully developed flow in a rod bundle. The geometry
303 of the bundle is taken from the OECD/NEA MATiS-H benchmarking experiment (Smith et al., 2013) in
304 which the test section consists of a 5×5 rod bundle enclosed in a square housing. The geometrical features
305 of the experimental rig are very similar to a real PWR fuel assembly, although the overall size is about
306 three times bigger than the latter. Figure 4 shows some details of the cross section of the rod bundle. The
307 working fluid used in the experiment is water at a bulk temperature T_0 of 35 °C, an operating pressure of
308 1.5 bar, and a bulk velocity u_0 of 1.5 m/s, corresponding to a Reynolds number of 50,250. In the original
309 experiment, no heating was applied to the rods. In the simulation, however, we impose a 200 kW/m^2
310 heating to the surface of the rods to evaluate the behaviour of SubChCFD for heat transfer predictions.
311 For the sake of simplicity, we assume that the density change due to temperature rise is negligible so that
312 the momentum transport is not strongly coupled with heat transfer. In order to assist the validation process,
313 a resolved CFD model has also been created for the same geometry to provide reference results in addition
314 to the experimental data including data for heat transfer. The computing mesh and the filtering mesh of
315 the rod bundle used in SubChCFD are shown in Figures 5 (a) and (b), respectively. It should be noted that
316 the computing mesh is generated based on Mesh-1 described in Figure 3. Figure 5 (c) is the mesh used in
317 the reference resolved CFD model. Since the flow inside the rod bundle is a wall-bounded shear flow, the
318 standard k-ε turbulence model and the scalable wall function are sufficient to produce reliable reference
319 results.

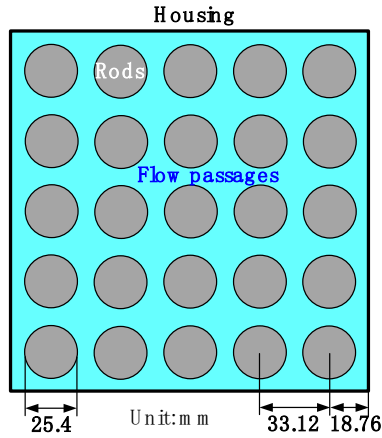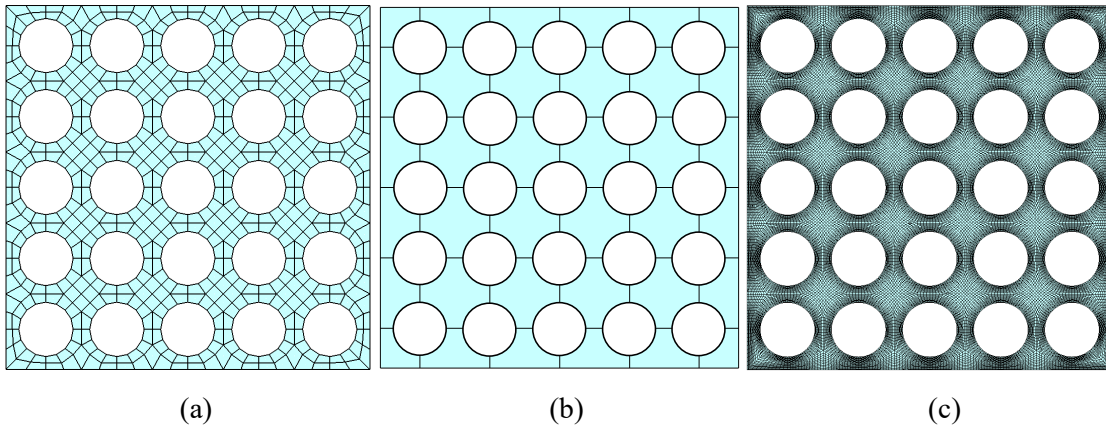Fig. 4 Sketch of the 5x5 rod bundle

| (a) | (b) | (c) |

Fig. 5 Meshes used in the simulation, including (a) the computing mesh of SubChCFD, (b) the filtering mesh of SubChCFD, and (c) the CFD mesh of the reference model

Considering the fact that the flow studied here is fully developed in the axial direction (also called stream-wise direction), periodic conditions are imposed to the boundaries perpendicular to the rods and only one layer of cells is used in the stream-wise direction, which makes the model effectively 2-D. For momentum, full-slip wall boundaries are enabled by applying zero-gradient conditions to all the solid walls, whereas an empirical correlation of the frictional factor

$$f = \left[a + b_1 \left(\frac{P}{D_h} - 1 \right) + b_2 \left(\frac{P}{D_h} - 1 \right)^2 \right] / \operatorname{Re}^n \qquad (10)$$

is used to calculate the wall friction which is further imposed as a momentum source term to the wall adjacent cells to account for the wall shear effect.

334   Table 2 gives the values of the parameters in the friction factor correlation for different types of sub-

335   channels in a square-lattice rod bundle (Todreas and Kazimi, 1990).

336   **Table 2 Parameters in the frictional factor correlation for square-lattice rod bundles**

Sub-channel type	a	b_1	b_2	n
Interior (laminar)	35.55	263.7	-190.2	1
Edge (laminar)	44.40	256.7	-267.6	1
Corner (laminar)	58.83	160.7	-203.5	1
Interior (turbulent)	0.1339	0.09059	-0.09926	0.18
Edge (turbulent)	0.143	0.04199	-0.04428	0.18
Corner (turbulent)	0.1452	0.02681	-0.03411	0.18

337

338   An energy sink term is introduced to the energy equation to continuously remove a certain amount of heat

339   which is in balance with that generated by the fuel rods so that a steady-state temperature field can be

340   finally obtained. The energy sink is based on the computing mesh and can be calculated as follows,

341
$$S_E = \frac{\Phi_{net}\vec{u}\cdot\vec{e}_z}{\int_{\Omega_d} \vec{u}\cdot\vec{e}_z dV} \qquad \frac{\Phi_{net}u_z}{\int_{\Omega_d} \vec{u}_z dV} \tag{11}$$

342   where Φ_{net} is the net heat input to the fluid, $\vec{e}_z$ is the unit vector of the stream-wise direction, Ω_d represents

343   the whole computational domain.

344   Since the Neumann type thermal boundary condition is used for all the solid walls in this case, as discussed

345   in Section 2, the Nusselt number does not enter the main simulation loop and is only used at the post-

346   processing stage to estimate the surface temperature of the fuel rods. The wall temperature is calculated

347   based on the filtering mesh using the following equation,

348
$$T_w = T_b - \frac{qD_h}{\lambda \text{Nu}} \tag{12}$$

349   The Nusselt number correlation used here for the rod bundle is derived as a product of $(\text{Nu}_\infty)_{c.t.}$ for the

350   circular pipe in fully developed conditions multiplied with a correction factor (Todreas and Kazimi, 1990).

351
$$\text{Nu} = \psi (\text{Nu}_\infty)_{c.t.} \tag{13}$$

352 where $\psi = 1 \quad 0.9120\,\mathrm{Re}^{-0.1}\,\mathrm{Pr}^{0.4}(1 \quad 2.0043e^{-B})$, $B=D_h/D$.

353 $(\mathrm{Nu}_\infty)_{\text{c.t.}}$ is given by the Dittus-Boelter equation (Dittus and Boelter, 1985),

354
$$(\mathrm{Nu}_\infty)_{c.t.} = \begin{cases} 0.023\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.4} & \text{when the fluid is heated} \\ 0.023\,\mathrm{Re}^{0.8}\,\mathrm{Pr}^{0.3} & \text{when the fluid is cooled} \end{cases} \tag{14}$$

355 3.1.2 Standard geometry with uniform heating (base-line validation case)

356 Figure 6 shows the simulation results of SubChCFD and resolved CFD for the 5×5 rod bundle. It can be
357 seen that SubChCFD is capable of capturing the main features of the velocity and temperature fields in
358 the sub-channels really well. It is also clear that SubChCFD does not show the stagnation and the hot
359 spots close to the wall predicted by the resolved CFD. This is expected because of the nature of this
360 approach. Figure 7 provides a more detailed comparison using line plots, in which experimental data are
361 also provided where available. It is first noted that the resolved CFD seems to overpredict the velocity
362 variation between the rods measured in the experiment. The results of the SubChCFD model follow very
363 closely these of the resolved CFD and also over-predict the temperature variations. Consequently, both
364 models can successfully capture the overall trend of the flow pattern but both of them have similar
365 deviations from the experimental measurements.

366

367 (a)   (b)
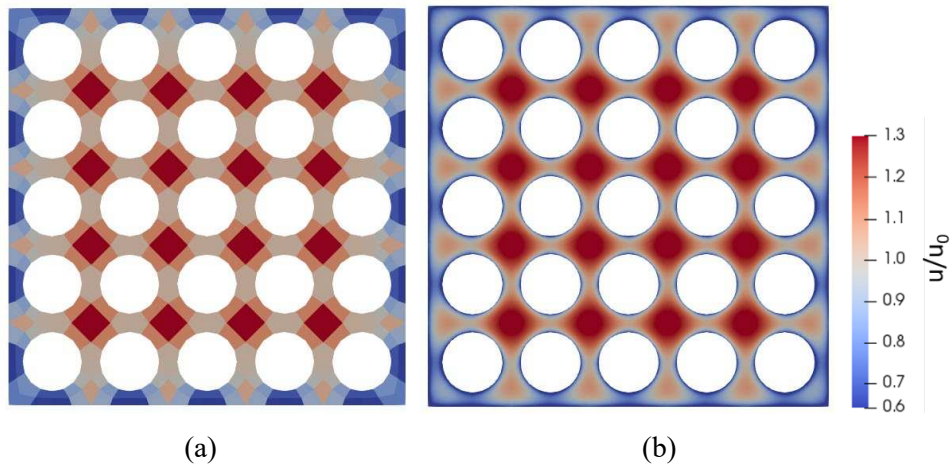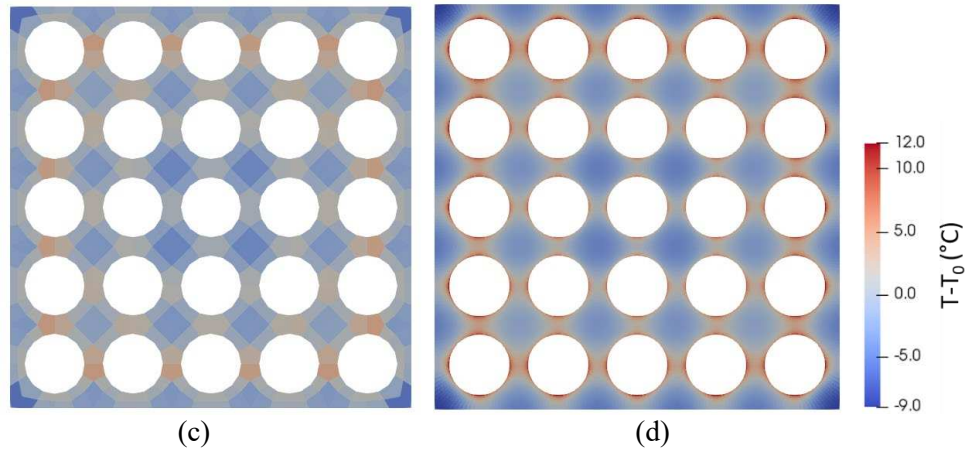
Fig. 6 Contour plots of the 5×5 bundle, (a) and (b) the normalised axial velocity distribution derived from SubChCFD and resolved CFD simulations, (c) and (d) the temperature distribution derived from SubChCFD and resolved CFD simulations
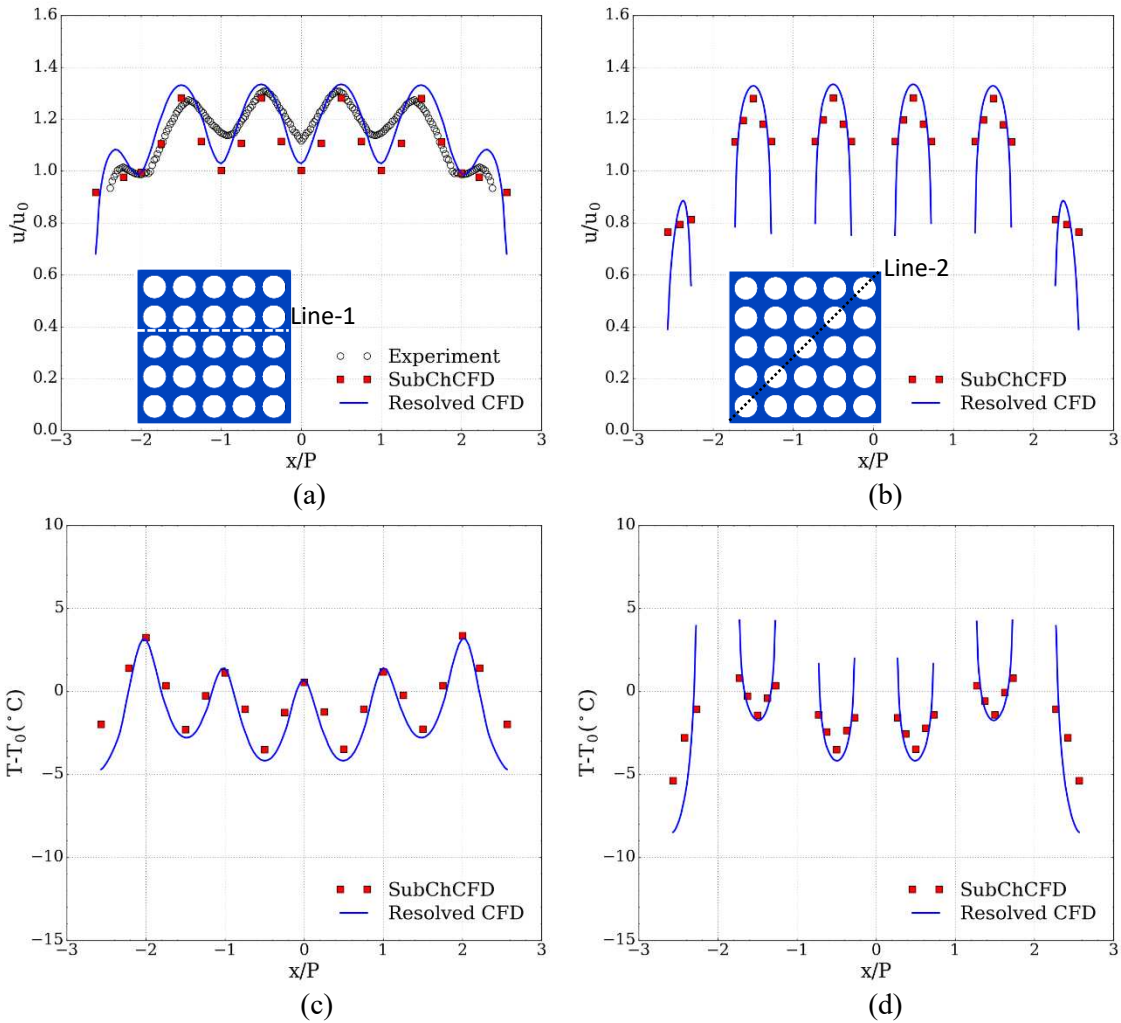
Fig. 7 Line plots of the 5x5 bundle, (a) and (b) the normalised axial velocity over line-1 and line-2, (c) and (d) temperature over line-1 and line-2
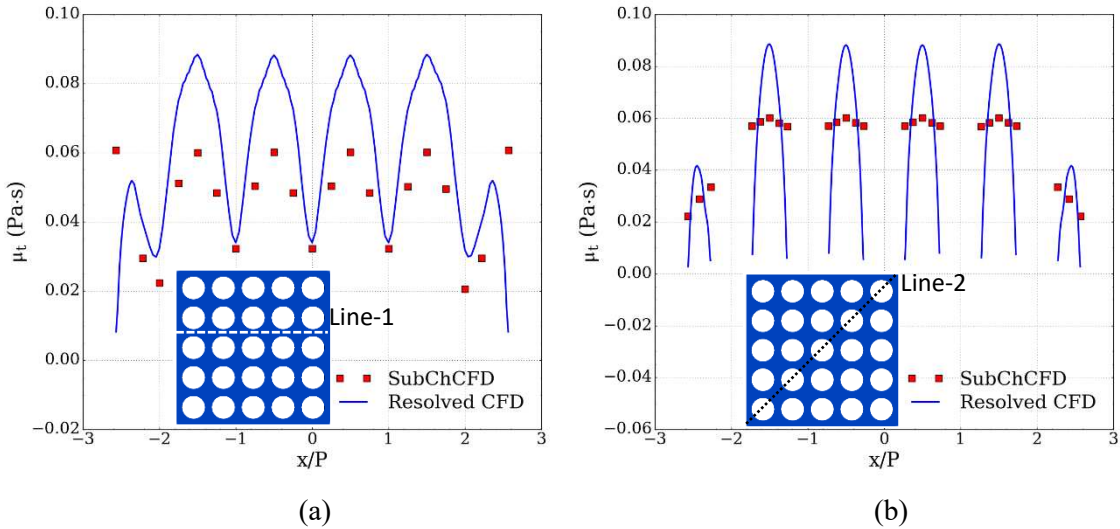
Fig. 8 Line plots of the turbulent viscosity over (a) line-1 and (b) line-2

The good agreement between SubChCFD and the resolved model in capturing much of the details of the flow away from the wall implies that the mixing length model is capable of predicting a correct level of turbulence in the core region of the sub-channels using a very coarse grid. Figure 8 shows a comparison between the turbulent viscosities predicted by the two methods along the same lines where the velocity and temperature are plotted. Overall, SubChCFD gives very good results compared to the resolved model especially on line-2, where it reproduces the average value of the latter rather well. On line-1, SubChCFD seems to under-predict the turbulent level compared to the resolved model, but it is insignificant and has little effects on the overall flow field.

Figure 9 shows the circumferential distribution of the rod surface temperature. Fuel rods at four representative locations (including a corner rod, an edge rod and two interior rods) are selected for plotting the results. It is clear that each rod in the array belongs to four adjacent sub-channels simultaneously. Therefore, the calculation of the surface temperature of a fuel rod for a complete 360º is segmented, depending on four different sub-channel bulk temperatures. This is the reason why the SubChCFD result has a stepwise variation along the azimuthal direction. For better comparison, trend lines are added for the resolved CFD results by applying a box filter to spatially average the original data. It can be noted that SubChCFD cannot capture every detail of the surface temperature on the fuel rods as that in a typical resolved CFD simulation. However, the basic trends of the surface temperature distribution can be qualitatively predicted, even though there is a shift between the predictions of the two methods. Considering that the bulk temperature predictions are similar in the two methods, this shift implies that the Nusselt number correlation used in the SubChCFD does not agree well with the heat transfer predicted by the resolved model. The difference is moderate, between 10 to 20% of the wall-to-bulk temperature

403 difference. It should be noted that the correlation used in this case study is one of a generic form
404 (Equations 13 & 14). In practice, the correlations used in SubChCFD are expected to be specifically
405 developed for the particular fuel designs concerned. Ideally, such correlations will be derived from
406 experiments, but more recently, CFD simulations have been used to extend the range of conditions of the
407 database produced from experiments with reasonable success.

408
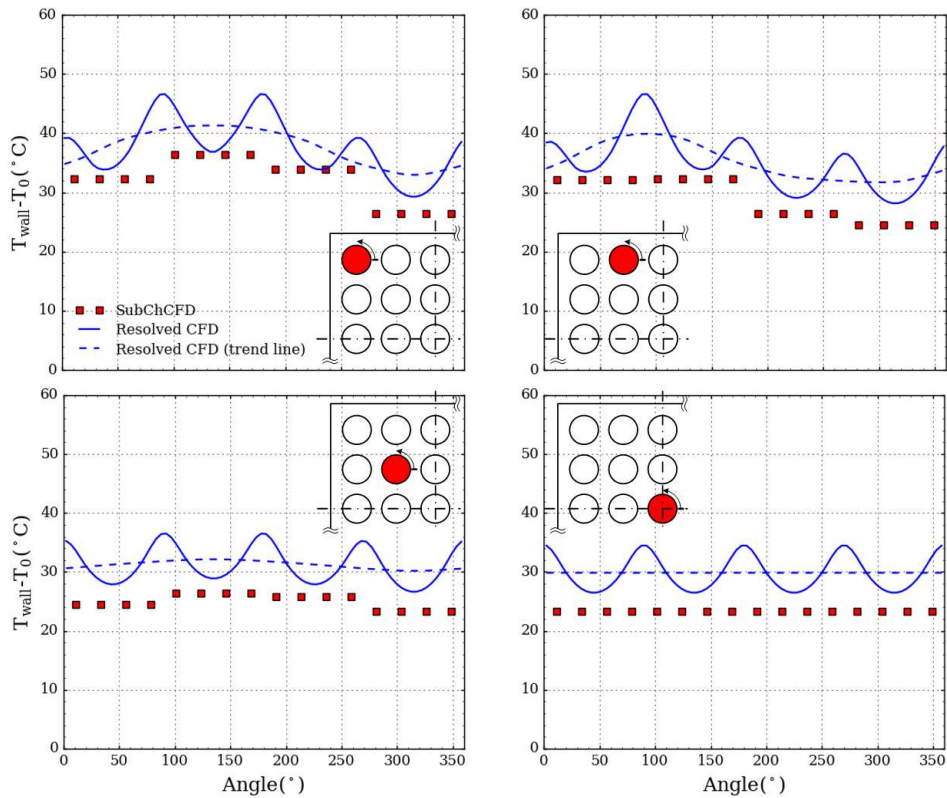
409

410 **Fig. 9 Circumferential distribution of the surface temperature of the rods at representative locations.**
411 **(The rod where the results are taken for plotting being highlighted in red)**

412 A basic concern of the methodology developed for SubChCFD is the use of a standard CFD solver on a
413 very coarse mesh, which may potentially cause significant discretisation error and consequent numerical
414 diffusion. In order to evaluate the mesh-dependency of SubChCFD, two other computing meshes, based
415 on resolutions of Mesh-2 and Mesh-3 (see Figure 3) respectively, are used to simulate the flow and heat
416 transfer in the base-line case. The results are shown in Figure 10 and compared with the Mesh-1 result. It
417 is interesting to observe that the results are nearly mesh independent although the Mesh-1 result slightly
418 deviates from the other two meshes in some regions of the edge sub-channel and the corner sub-channel.
419 Overall, the three meshes produce very similar results in terms of both velocity and temperature fields,
420 which is especially the case for Mesh-2 and Mesh-3 results. This suggests that the numerical diffusion

421   related to the coarse mesh plays a relatively small role for this type of wall-bounded shear flows. However,

422   it could be very significant in other cases and needs to be quantified wherever necessary in the future.
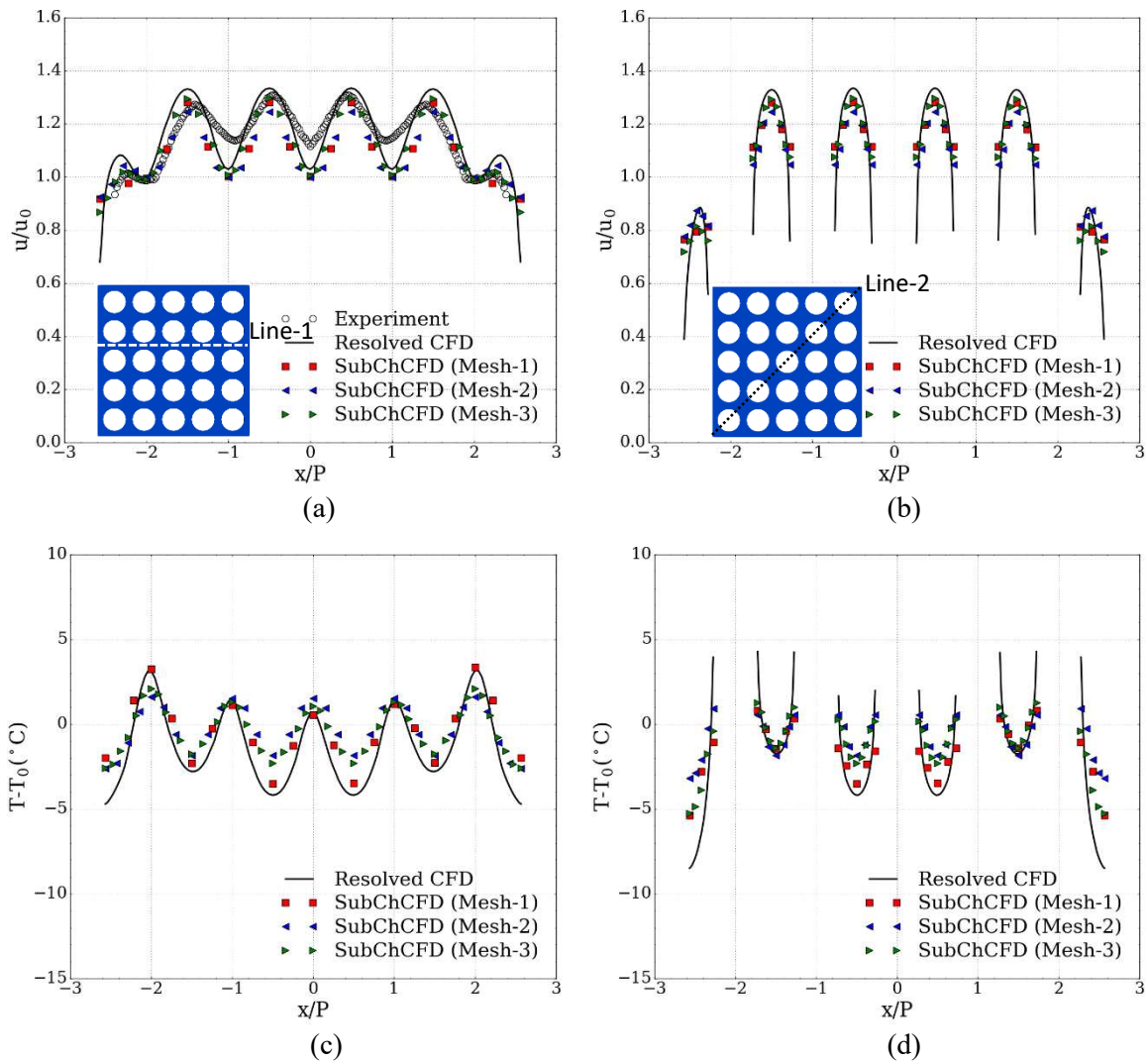
Fig. 10 Mesh-dependency test, (a) and (b) the normalised axial velocity over line-1 and line-2, (c) and (d) temperature over line-1 and line-2

429   To roughly compare the computing costs of SubChCFD and resolved CFD, serial simulations (using only

430   1 CPU processor) were run using the two methods, respectively, for a certain length of physical time at a

431   fixed CFL number. Results obtained can be found in Table 3. As can be seen, the mean elapsed time per

432   time step of SubChCFD is about only 1/60 that of resolved CFD due to the significant reduction in mesh

433   size. Additionally, larger time step size is allowed at the same CFL number in SubChCFD because the

434   local size of the mesh cells is larger, which results in an extra reduction in computing cost compared to

435 resolve CFD. Overall, the computing cost is saved by up to 560 times by using SubChCFD in this
436 particular case.

437 **Table 3 Evaluation of computing costs of Resolved CFD and SubChCFD**

Method	Mesh size (number of cells included)	Mean elapsed time per time step (s)	Mean time step size (s)	Elapsed time per physical time (s/s)
Resolved CFD	54,528	0.6369	0.001	636.9
SubChCFD	1,120	0.01184	0.0104	1.138

438

### 3.1.3 Standard geometry with non-uniform heating

440 To further assess the performance of SubChCFD, simulations have been carried out for two additional
441 flow scenarios derived by altering the distribution of the heating source and the geometrical layout of the
442 rods of the base-line validation case.

443 The first case is aimed at testing the performance of SubChCFD when applied to non-uniformly heated
444 bundles. This occurs in reactors, for example, following refuelling when fresh fuel sits next to the
445 boundary of partially spent fuel assemblies. For the sake of simplicity, a non-uniform thermal
446 environment is created in this test case by imposing a 200 kW/m^2 heat loading to the centre rod with all
447 other rods being teated as adiabatic. The flow condition in this case is exactly the same as that used in the
448 base-line validation case, so the velocity fields of the two cases are expected to be identical because there
449 is no feedback from the changed heat transfer circumstances to the momentum transport due to the use of
450 constant fluid physical properties. Hence, only the temperature results are presented in this section.
451 Figures 11 and 12 show the resulting temperature field predictions in forms of contour and line plots,
452 respectively. It can be seen that the temperature distribution predicted by SubChCFD agrees well with
453 that exhibited in the results of the resolved CFD in this non-uniform heating scenario. The large
454 temperature variations within the sub-channels adjacent to the heated rod are well captured by SubChCFD.
455 This is unlikely to be achieved using a traditional sub-channel code. In addition, the resolution of the
456 results can be controlled, to some extent, by employing different computing meshes. In this sense,
457 SubChCFD performs as flexible as a typical CFD approach.

458

459   (a)   (b)
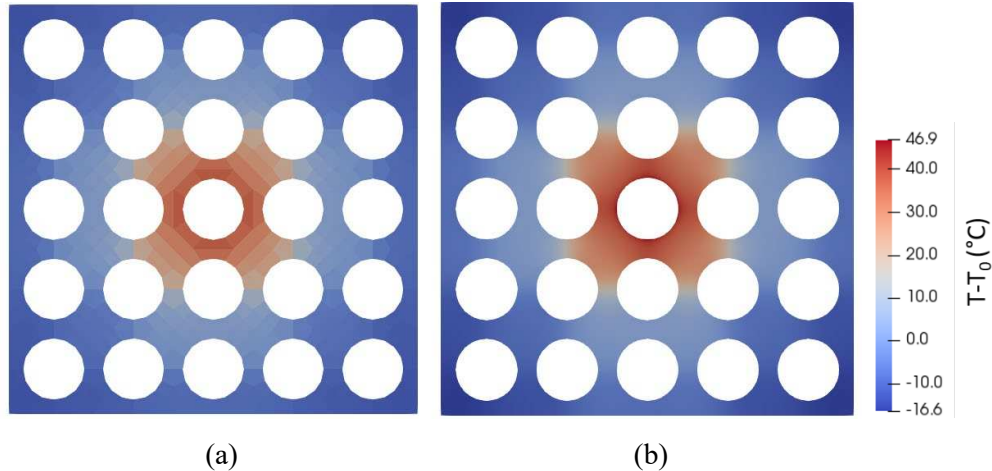
460   **Fig. 11 Temperature distribution of non-uniformly heated bundle obtained with (a) SubChCFD and**

461   **(b) resolved CFD**

462

463   (a)   (b)
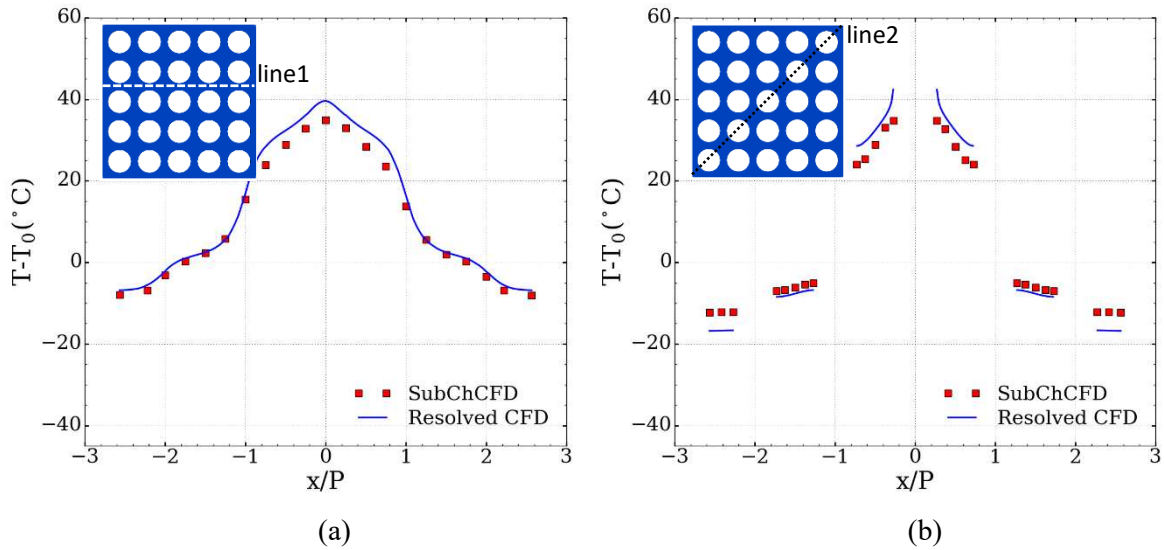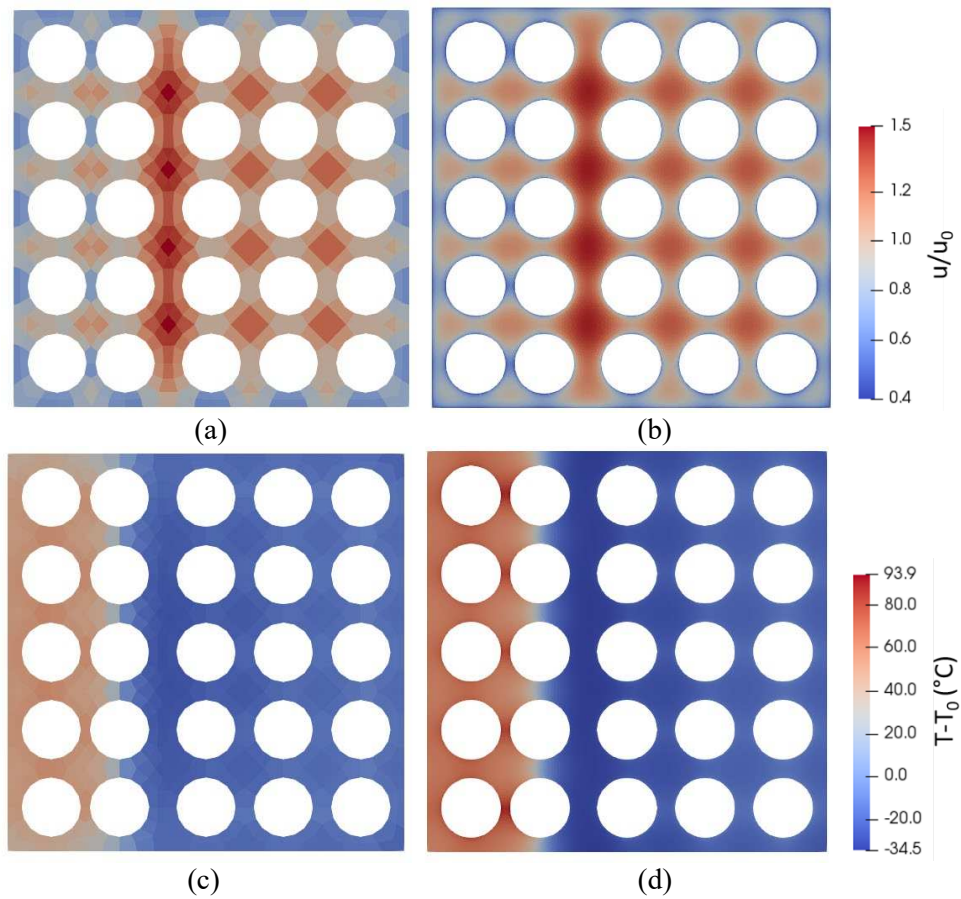
464   **Fig. 12 Line plots of the temperature field over (a) line 1 and (b) line2**

3.1.4 Distorted geometry with uniform heating

466   The second case is aimed at testing SubChCFD for geometrically distorted rod bundles, which is also of

467   great importance in engineering practice, especially for safety assessment. Here, we shift one column of

468   the rods slightly to one side, creating a widened and a narrowed sub-channel on the two sides, respectively.

469   The geometry change is expected to redistribute the mass flow among the sub-channels, leading to

470   significant non-uniformity of the temperature distribution. Figures 13 and 14 show the simulation results

471   of SubChCFD and the resolved CFD for the distorted rod bundle. It can be seen that SubChCFD responds

472   to the geometrical change very well in terms of flow redistribution. The temperature redistribution has

473   also been qualitatively captured, for example, the local increase in temperature caused by the reduction

474   of the coolant flow in narrow sub-channels, although the agreement could be further improved if required

475   by calibrating some of the model parameters, such as the turbulent Prandtl number.

476

477
       (a)   (b)

478

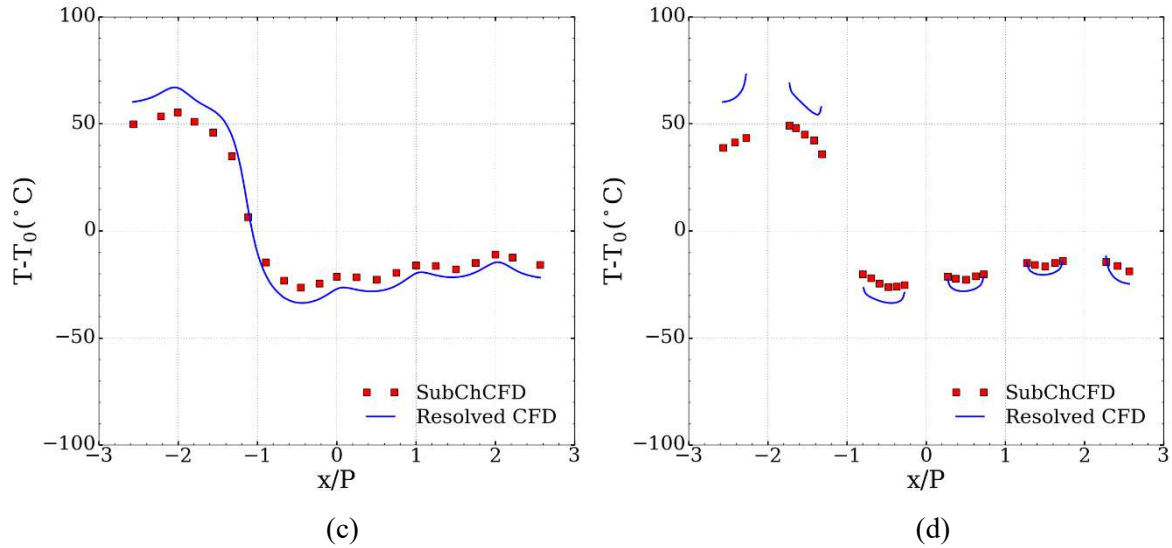479   (c)   (d)

480   **Fig. 13 Simulation results of the geometrically altered rod bundle, (a) and (b) the normalised axial**

481   **velocity fields, (c) and (d) the temperature fields**

482

483   (a)   (b)

484

485   (c)   (d)
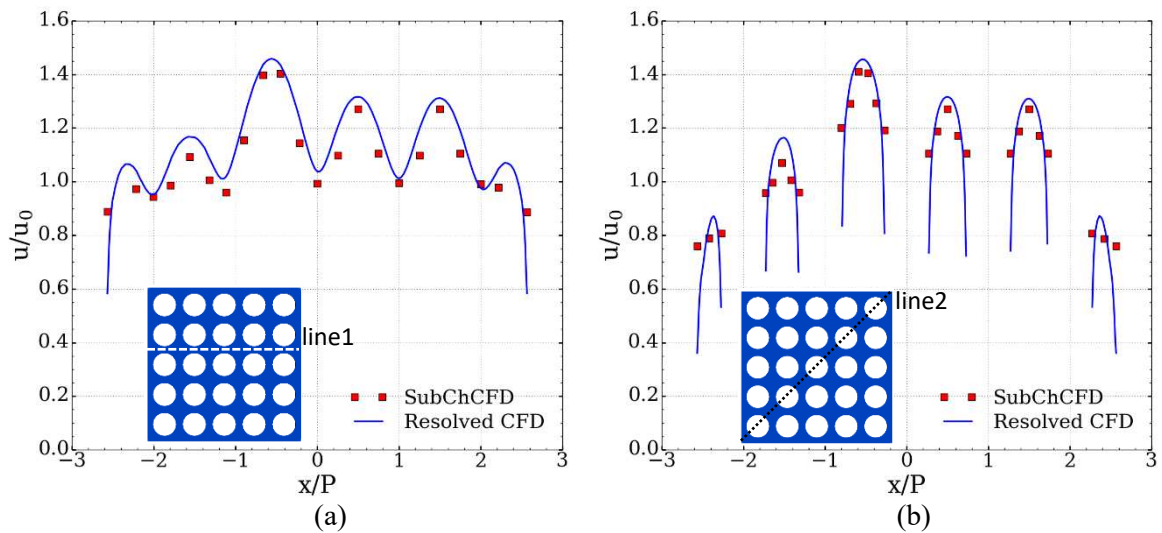
486   **Fig. 14 Line plots of the velocity and temperature fields, (a) and (b) the normalised axial velocity over**

487   **line 1 and line2, (c) and (d) the temperature over line 1 and line 2**

488   ## 3.2   Flow in a rod bundle with local blockage

489   The aforementioned test cases have demonstrated the feasibility of SubChCFD for calculations of fuel

490   bundle flow and heat transfer. It is not only able to predict sub-channel-level behaviours but also to capture

491   sub-scale physics within the sub-channels. Benefiting from the greatly reduced computing cost compared

492   to resolved CFD, SubChCFD can be used for simulation of large-scale reactor components. In this section

493   and the following one, we will further assess the performance of SubChCFD for full 3-D large-scale

494   bundle flows.

495   The following case is used to test the capability of SubChCFD in tackling non-design operating

496   circumstances. It is created by positioning a blockage in one of the sub-channels to obstruct the flow at a

497   certain height in a 5×5 rod bundle. Geometrical details of the obstruction can be found in Figures 15 (a)

498   and (b). During the operations in nuclear reactors, partial or complete blocking of single or multiple sub-

499   channels of the reactor core is considered to be a credible scenario, for example, in PWR reactors due to

500   LOCA-related rod swelling or ballooning (Creer et al., 1976). Due to the local blockage, the nearby

501   coolant flow is significantly distorted, resulting in locally strengthened inter-channel mixing and lateral

502   flow. The traditional sub-channel codes would find this very challenging due to the restrictions of the 1-

503   D framework of formulation used. Some special treatment might be developed but it is impossible for

504   such an approach to describe the 3-D flow phenomenon around the blockage and the large scale

505   recirculation downstream in any detail. In contrast, SubChCFD is naturally suitable for this type of

506   problem. Figure 15 (c) shows the extruded mesh of a cross-section passing through the blockage region,

507 which is generated based on the resolution of computing Mesh-2 described in Figure 3. The total amount

508 of hexahedral cells for the entire 3-D SubChCFD model is about 0.645 million. This is much lower than

509 that used in the CFD reference model which consists of as many as 21 million hexahedral mesh cells.

(a)   (b)   (c)
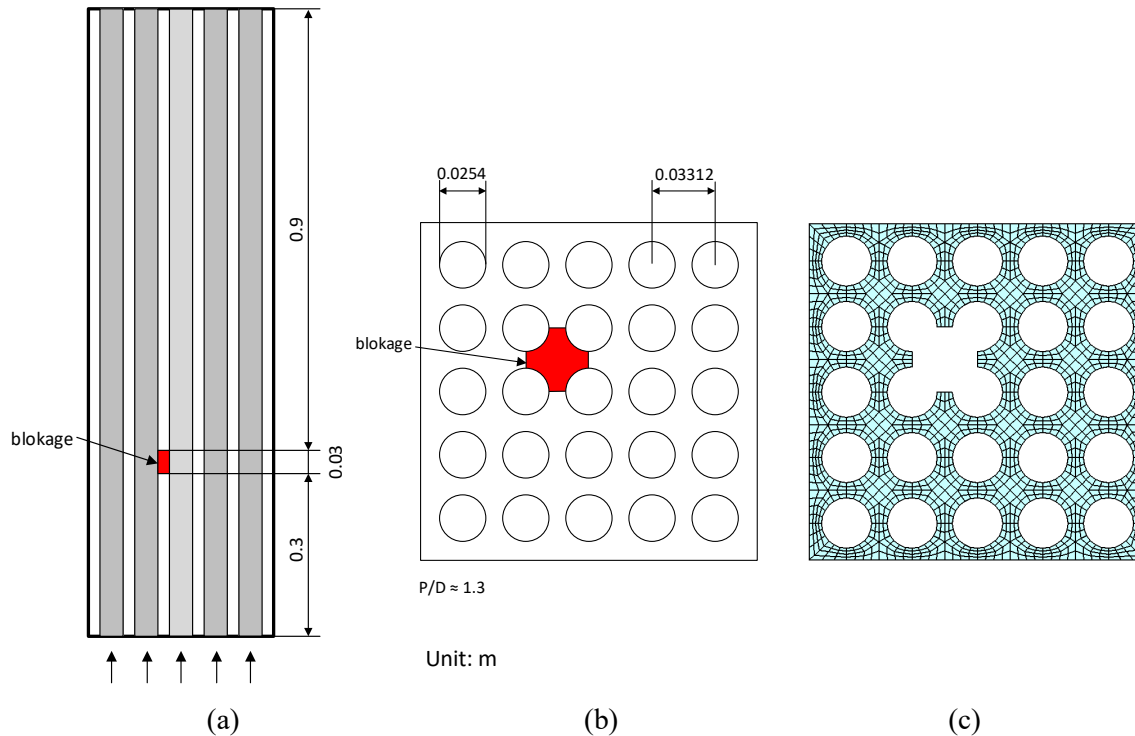
Fig. 15 Geometry and mesh of the 3-D rod bundle with local blockage, (a) and (b) the longitudinal and the cross-section view of the rod bundle (unit in m), (c) a cross-section of the computing mesh used in the SubChCFD model

515 Figure 16 shows comparisons between the simulation results produced using SubChCFD and the resolved

516 CFD. The x-component of the cross-flow velocity is firstly plotted along a horizontal line (i.e. line-1 in

517 Figure 16 a), which reflects the profile of the lateral flow distribution around the blockage area. It can be

518 seen that SubChCFD produces very similar result to that of the resolved CFD. In this region, the

519 Bernoulli's effect plays a leading role in shaping the local flow around the blockage, which can be just

520 properly captured by SubChCFD. There are pressure losses due to re-circulation around the blockage,

521 which are not currently modelled in SubChCFD. This lack does not affect the results significantly here,

522 but the pressure losses could be accounted for in the model in the future. Figure 16 (c) shows the pressure

523 distribution along line-2 shown in Figure 16 (a). As can be seen, the overall trend of the pressure variation

524 is captured but some details, such as the appearance of the lower peak, cannot be reproduced with the

525 SubChCFD simulations. Figure 16 (d) shows the axial pressure distribution along the centre line of sub-

526 channel A (the sub-channel on the right-hand side close to the blockage, see sub-Figure 16 a). It is worth

527   noting that SubChCFD agrees very well with the resolved CFD in predicting the frictional loss of the non-
528   blocked section and form loss of the blocked section, even though the local peak value is not accurately
529   captured in comparison to the resolved simulation results. The sharp pressure dips are linked to the rapid
530   local flow acceleration due to the reduced area. This is an inviscid effect and the pressure recovers and
531   the velocity returns to its original value past the restricted flow area region, which explains why this effect
532   is not captured by SubChCFD accurately, however, this sharp change, does not affect its overall
533   performance.

(a)

(b)

(c)

(d)
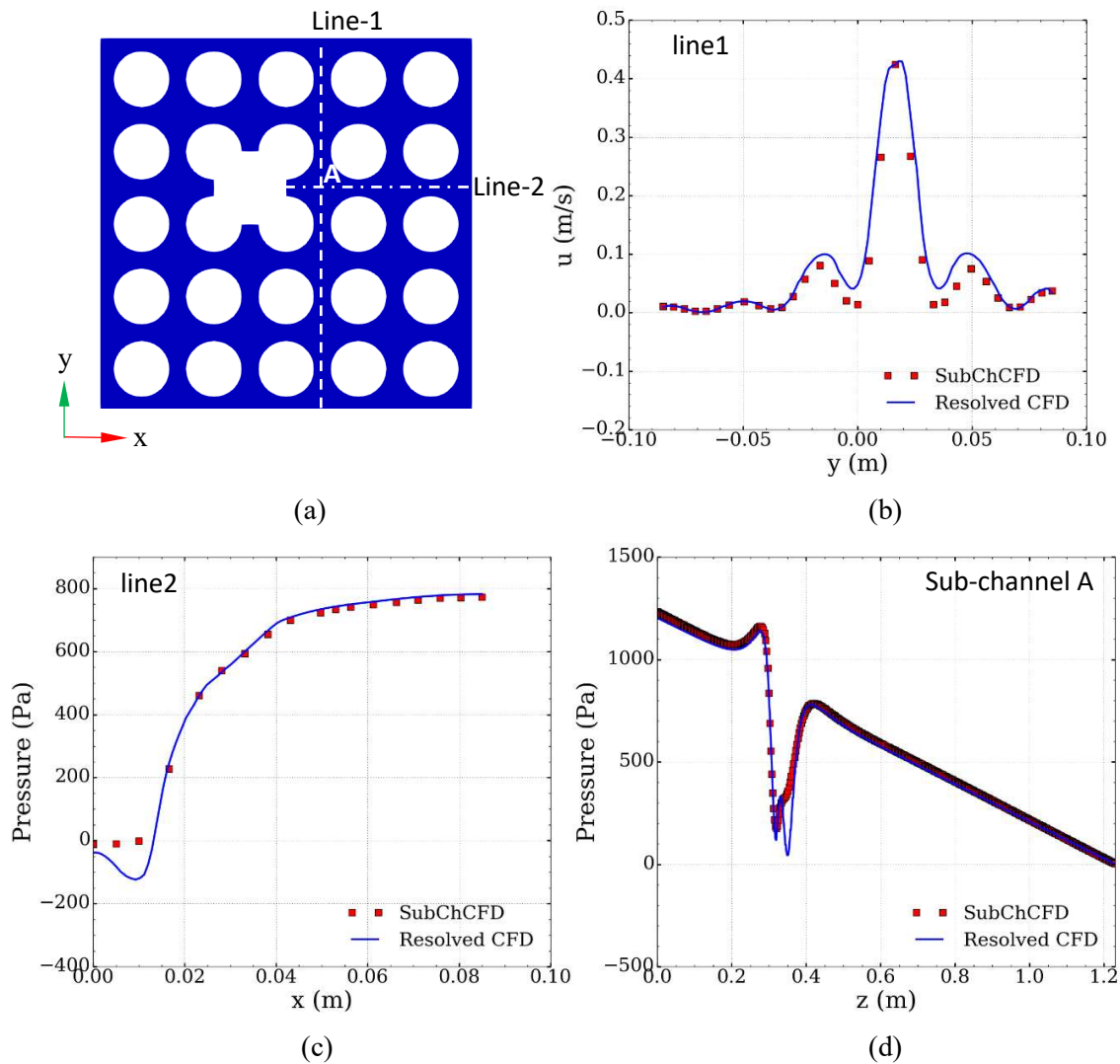
Fig. 16 Simulation results of the 3-D bundle with local blockage, (a) position of lines for plotting, (b) the x-direction velocity alone line-1, (c) the transverse pressure distribution alone line-2, (d) the axial pressure loss in sub-channel A

541   The computing cost was estimated in a similar way as that used in Section 3.1.2. However, simulations

542   were not conducted in a serial manner due to the relatively large mesh size used in this case. Instead, they

543   were run on a high performance computing (HPC) cluster. Considering the fact that the parallel speed-up

544   of using Code_Saturne is in linear with the number of CPU processors, providing that each partition has

545   no less than 10,000 to 20,000 cells (which is the case in the current investigation), the CPU time can be

546   easily converted to an equivalent elapsed time of using only one processor. As such, the computing costs

547   were estimated for both SubChCFD and resolved CFD, in which the former is about 190 times lower than

548   the latter. It should be pointed out that the reduction in computing cost in such a full 3-D case is even

549   lower than that of a 2-D case (see Section 3.1.2). This is mainly due to the use of a higher resolution mesh

550   (Mesh-2 in Figure 3) for the SubChCFD simulation.

3.3   Flow in a two-parallel-assembly

552   The experimental test of flow in a two-14×14 parallel-assembly was carried out by Weiss and Markley

553   (1971), aimed at investigating the flow redistribution between two open fuel assemblies resulting from a

554   partial or full blockage at the entrance of one assembly. This case has also been studied numerically by

555   S.J. Yoon et al. (2017) using their newly developed sub-channel code CUPID. This is a perfect case for

556   direct comparisons between SubChCFD and the sub-channel codes used in large-scale component

557   modelling.

558   The test section of the experimental rig consists of two 14×14 fuel assemblies interconnected through a

559   water gap and enclosed in a rectangular housing (see Figure 17). Each of the assemblies is 0.1869 m in

560   width and 0.1938 m in height, and the width of the water gap is 0.0155 m. The diameter of the rods is

561   0.0108 m and the pitch-to-diameter ratio is 1.28. The fuel assembly on the right-hand side is assumed to

562   be partially blocked at the entrance, resulting in a reduced mass flux compared to the left assembly. In the

563   numerical simulation, to reproduce the mass flow rates of 550 g/min and 1,110 g/min for the two bundles,

564   inlet bulk velocities are set to 1.76 m/s and 3.52 m/s, respectively. For the water gap, the inlet velocity is

565   assigned as 2.64 m/s.

566   Figure 18 shows the cross-section view of the computing mesh used for the parallel fuel assembly based

567   on the resolution of Mesh-1 described in Figure 3. As can be seen from the zoomed-in inset, the

568   distribution of the grid lines has been adjusted slightly in the edge sub-channels to improve the quality of

569   the mesh elements close to the wall. Based on such resolution, a 3.3 million hexahedral cell mesh was

570   generated for the entire 3-D model. A resolved CFD simulation for this case would need about 400 million

571   cells, which is a large model even for current Tier-1/Tier-2 HPC research facilities. Instead of conducting

572   a resolved CFD simulation, we evaluate the results of the SubChCFD by comparing them with those

573 obtained from the sub-channel code CUPID and the available experimental data. Figure 19 shows the
574 axial velocity profiles at six different vertical elevations of the parallel assembly. They are plotted using
575 mean values calculated through arithmetic averaging at three sampling locations in accordance to the
576 experimental measuring points, located at the centre lines between row-2 and row-3, row-7 and row-8,
577 and row-12 and row-13 of the fuel rods, respectively. For most of the levels (except level 2), the
578 SubChCFD results agree somewhat better with the experimental data than those produced by CUPID.
579 Moreover, as expected, SubChCFD provides more details of the flow profile than the traditional sub-
580 channel code. For instance, the variation of the axial velocity occurring between the gap and the centre of
581 the sub-channel are well captured. These variations appear to be smaller nearer the mixing interface as
582 expected, where the strong cross flow and mixing smooth out the velocity gradients. Such phenomena
583 cannot be predicted using a traditional sub-channel code.
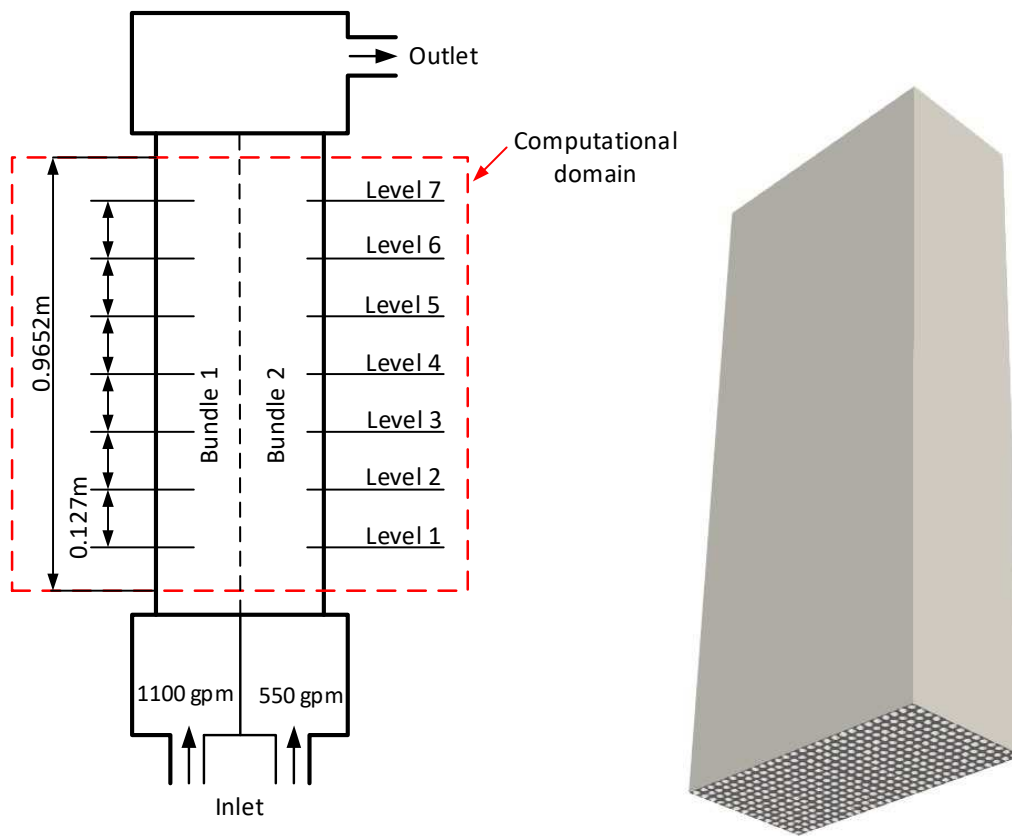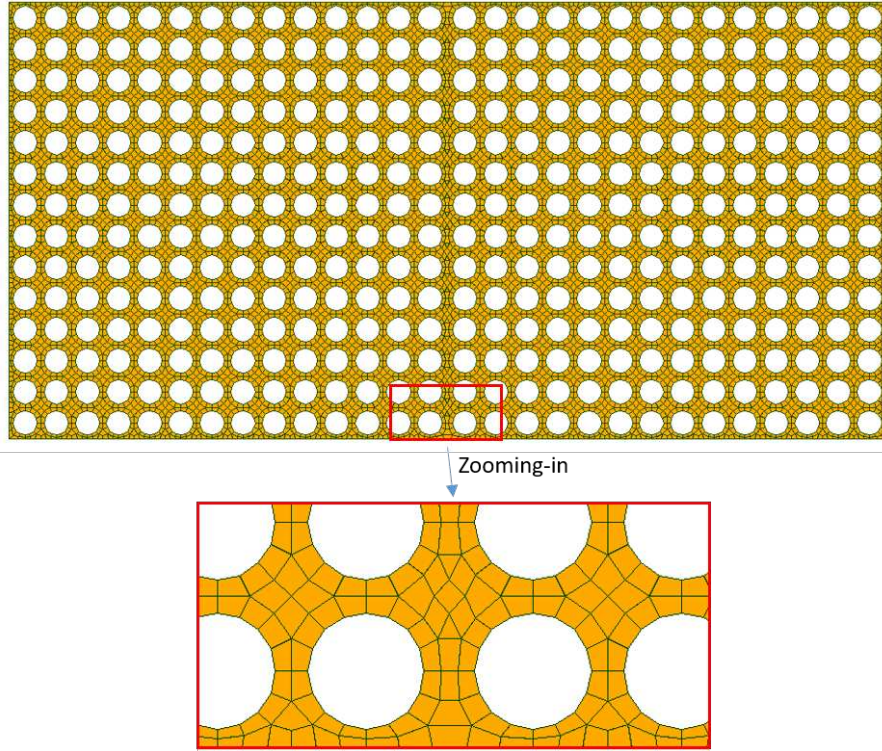

584
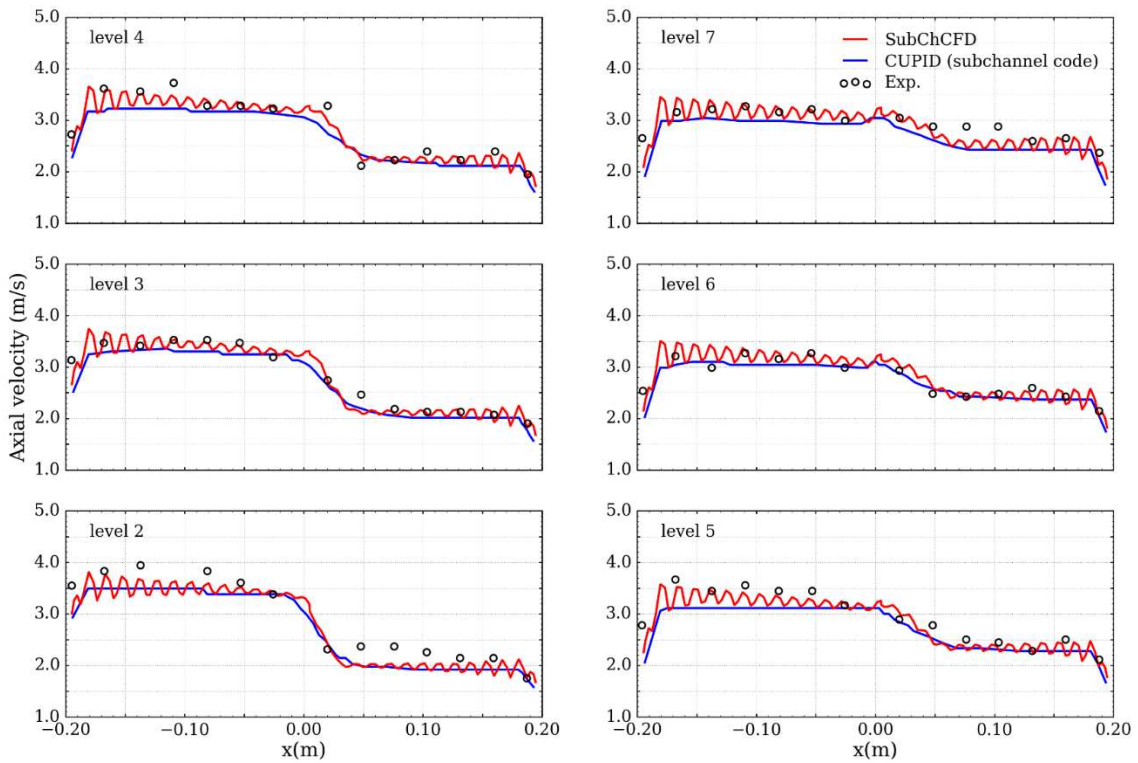585 (a) (Yoon et al., 2017) (b)
586 **Fig. 17 Modelling of the parallel fuel assembly, (a) schematic of the experimental facility, (b) numerical**
587 **model of the test section**

588

Fig. 18 Cross section view of the computing mesh for the parallel assembly

590

Fig. 19 Axial mean velocity profiles of the parallel assembly

4. Conclusions

A coarse-grid CFD-based, modern, sub-channel methodology (SubChCFD) has been developed to bridge the gap between the system/sub-channel codes and the conventional CFD. The convection term is directly discretised on the coarse mesh and the diffusion term is split into two parts, including the wall-boundary part and the interior part, respectively. The latter is then described using a simple turbulence model (a 0-equation mixing length turbulence model in this paper), whilst the former is tackled in a similar way as that is normally done in a sub-channel analysis code, using empirical correlations as closure laws. In doing so, on one hand, the computing cost is significantly reduced compared to conventional CFD methods due to the use of a coarse mesh, making it possible to simulate large reactor components or even the whole core. On the other hand, some advanced features of the conventional CFD are retained, including a full 3-D solution, high simulation robustness and application flexibility. SubChCFD can be readily coupled with resolved CFD or any other CFD-based methods (e.g. porous media approach), which is an important feature of this method. The former enables flexible local refinement in regions where the sub-grid flow phenomena are of interest. The latter can be used as a simple treatment of complex internal structures, such as spacer grids. Both will be explored as a follow-up of this work.

The methodology of SubChCFD has been implemented into the open-source CFD package Code_Saturne. A numerical test has then done for the 5×5 bare bundle of the OECD/NEA MATiS-H benchmarking experiment. It has been shown that SubChCFD has good numerical stability and robustness, and is able to capture the flow and heat transfer well in this axially dominant bundle flows, with a significant reduction in computing cost compared to conventional CFD.

Next, SubChCFD has been used to simulate two complex 3-D flow cases. The first case is a locally blocked rod bundle derived by placing an obstruction in one of the sub-channels. The cross-flow due to the blockage has been well captured and the predicted axial pressure loss due to friction and obstruction are in good agreement with those obtained from a resolved CFD simulation. The second case comprises two parallel fuel assemblies with different input mass flow rates. In this case, SubChCFD also produces excellent predictions, not only by successfully capturing the distribution of the axial velocity due to the inter-channel mixing but also by providing flow details within sub-channels which cannot be captured by the traditional sub-channel codes. In the future, SubChCFD will be further developed to broaden the scope of its application, including, for example, transverse-dominant flows, buoyancy-influenced mixed convection or natural circulation. Methods for coupling SubChCFD with resolved CFD and/or porous media method will also be explored.

624 Nomenclature

C_p	Specific heat, [J/(kg·°C)]
D	Rod diameter, [m]
D_h	Sub-channel hydraulic diameter, [m]
$\vec{e}_z$	Unit vector of the stream-wise direction
f	Skin frictional factor
$\overline{I}$	Unit tensor
l_m	The mixing length, [m]
$\vec{n}$	Outward normal vector of a cell surface
Nu	Sub-channel Nusselt number
$(Nu_\infty)_{c.t.}$	Nusselt number for a circular pipe at fully developed condition
p	Static pressure, [Pa]
P	Pitch of a rod array, [m]
Pr	Prandtl number
q	Heat flux of the rod surface, [W/m²]
Re	Sub-channel Reynolds number
S_w	Cell surface that is adjacent to a wall boundary, [m²]
S_f	Cell surface that is not adjacent to a wall boundary, [m²]
S	Total cell surface, $S = S_w \cup S_f$, [m²]
S_{ij}	Components of the strain rate tensor, [s⁻¹]
$\vec{S}_u$	Source term of the momentum equation, [N/m³]
S_E	Source term of the energy equation, [W/m³]
t	Time, [s]
T	Temperature, [°C]
T_0	Global bulk temperature, [°C]
T_b	Sub-channel bulk temperature, [°C]
T_w	Wall temperature, [°C]
$\vec{u}$	Velocity vector, [m/s]
u_0	Global bulk velocity, [m/s]
$\vec{u}_b$	Sub-channel bulk velocity vector, [m/s]
V_i	Volume of the ith computing mesh cell, [m³]
$V_{sub,j}$	Volume of the jth filtering mesh cell, [m³]

Greek symbols

Δ	Thickness of the boundary layer, [m]
δ	Kronecker notation
φ_i	CFD-level quantity of φ on the ith computing mesh cell
$\varphi_{sub,j}$	Sub-channel-level quantity of φ on the jth filtering mesh element
Φ_{net}	Net heat input to a flow domain, [J/s]
λ	Thermal conductivity, [W/(m·°C)]
λ_t	Turbulent thermal conductivity, [W/(m·°C)]
μ	Molecular viscosity, [Pa·s]
μ_t	Eddy viscosity, [Pa·s]
Ω	A cell of the computing mesh
Ω_d	The whole computational domain
Ω_{sub}	A cell of the filtering mesh

ρ		Fluid density, [kg/m^3]
$\overline{\sigma}$		Stress tensor, [Pa]
ψ		Correction factor of the Nusselt number for rod bundles

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