1 **Influence of VOF technique, turbulence model and discretization scheme on the numerical**
2 **simulation of the non-aerated, skimming flow in stepped spillways**
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4 Arnau Bayon,[1,*] Juan Pablo Toro,[2] Fabián A. Bombardelli,[3] Jorge Matos,[4] and Petra Amparo
5 López-Jiménez [5]
6 [1]Research Institute of Water and Environmental Engineering (IIAMA). Universitat Politècnica
7 de València, Camí de Vera, s/n, 46022, València, Spain (arbabar@iiama.upv.es)
8 [2]Assistant Professor, Department of Civil Engineering, Universidad Andres Bello, Santiago
9 8320000, Chile; formerly, Ph.D. Candidate, Department of Civil and Environmental Engineering,
10 Univ. of California, 2001 Ghausi Hall, One Shields Ave., Davis, CA 95616. E-mail:
11 juan.toro.l@unab.cl
12 [3]Department of Civil and Environmental Engineering, University of California, Davis, USA
13 (fabianbombardelli2@gmail.com)
14 [4]Department of Civil Engineering, Architecture and Georesources, Instituto Superior Técnico,
15 Universidade de Lisboa, Av. Rovisco Pais 1, 1049-001, Lisboa, Portugal
16 (jorge.matos@tecnico.ulisboa.pt)
17 [5]Department of Hydraulic and Environmental Engineering, Universitat Politècnica de València,
18 Camí de Vera, s/n, 46022, València, Spain (palopez@upv.es)
19 [*]Corresponding author

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21

22 **Abstract**

23

24 An accurate description of the hydrodynamics in the non-aerated region of the skimming flow on

25 stepped spillways is of outmost importance, particularly in small structures at large discharges. In

26 addition, the flow features upstream of the inception point of air entrainment determine the flow

27 behavior in the downstream self-aerated region. In this work, numerical models of the flow in the

28 non-aerated region of stepped spillways have been developed using diverse turbulence closures

29 and discretization schemes implemented in two CFD codes: *OpenFOAM* and *FLOW-3D*®. Partial

30 VOF (Volume of Fluid) and "True" VOF (*TruVOF*) approaches are employed to capture the

31 position of the free surface. The Standard, RNG and Realizable k-ε, in addition to the SST k-ω

32   model, are used for turbulence closure. Numerical results are compared against reference

33   experimental results obtained from a physical model of constant slope of 0.75H:1V. Models with

34   turbulence closures of the k-ε family provide nearly the same predictions for the mean flow

35   velocity with maximum differences on average smaller than 1%. Regarding discretization schemes,

36   the first-order upwind method provides predictions for the mean flow velocity which are not

37   significantly different (within 6%) than those obtained with second-order counterparts. However,

38   these differences can be larger when maximum values of turbulent kinetic energy (TKE) and

39   dissipation rate of TKE at the step edges are compared. In spite of the fact that the *TruVOF*

40   (*FLOW-3D*[®]) method does not account for the tangential stresses at the air-water interface,

41   differences in the tracking of the free surface position among this method and the Partial VOF

42   method (*OpenFOAM*) were found to be smaller than 3% along the stepped spillway. In this work,

43   we also provide a physical interpretation of the flow results.

44

45   **Keywords**: Stepped spillway; Computational Fluid Dynamics (CFD); *OpenFOAM*; *FLOW-3D*;

46   RANS; VOF.

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48   **1. Introduction**

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50   Stepped spillways have been used for centuries as multi-purpose hydraulic structures: flow

51   energy dissipation, aesthetics, flood evacuation, etc. (Chanson, 2002). It was not until last century,

52   in concomitance with the spreading of new construction methodologies, such as roller compacted

53   concrete (RCC), that stepped spillways became an appealing way to dissipate energy (Chanson et

54   al., 2015; Matos & Meireles, 2014).

55   The presence of macro-roughness elements increases the rate of boundary-layer development

56   in the stepped spillway, thus displacing upstream the inception point of air entrainment; i.e., the

57   section where the boundary layer encounters the water free surface and eddies possess enough

58   energy to distort it (Meireles et al., 2014).

59   So far, most of the studies in the literature have been based on experimental modeling in the

60   self-aerated, skimming flow region (see e.g., Chanson, 2002; Matos & Meireles, 2014; Chanson et

61   al., 2015). Such studies have been able to provide clear insight into relevant subjects, such as

62   location of the inception of air entrainment, air concentration and velocity distributions, pressure

63   distribution on the step faces, flow resistance and energy dissipation.

64   The quantity of studies dealing with the non-aerated part of the flow is limited (Amador, 2005;

65   Amador et al., 2006; Bombardelli et al., 2011; Carvalho & Amador, 2009; Hunt & Kadavy, 2010;

66   Meireles & Matos, 2009; Toro et al., 2016; Zhang & Chanson, 2016a, 2016b). This fact is to a

67   certain extent justified, as on most prototype applications self-aeration would occur in a

68   considerable portion of the chute for the design discharge. Nevertheless, in some real-life cases,

69   especially in small structures at large discharges, the non-aerated flow can dominate most of the

70   length of the flow (Bombardelli et al., 2011; Meireles et al., 2014). Characterizing the non-aerated

71   region of the flow is also important with regard to cavitation. Recent studies showed that if flow

72   velocities in the non-aerated skimming flow region are large enough, cavitation and related

73   damage on the step surfaces may occur (Frizell et al. 2013, 2015). In addition, an accurate

74   description of maximum velocities and turbulence statistics close to the inception point of air

75   entrainment is crucial for the understanding of the flow features downstream of the inception point

76   (Toro et al., 2016). To the best of the Authors' knowledge, a full and comprehensive description of

77   the flow features in the aerated zone has not been achieved so far.

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78   Recent numerical works focusing on the non-aerated region have provided good predictions of

79   time-averaged velocities, water depths, development of the boundary layer and turbulence statistics

80   (Bombardelli et al., 2011; Meireles, 2011; Toro et al., 2016). However, relatively little emphasis

81   has been put into the influence of the VOF technique, the turbulence closure and the discretization

82   schemes on the numerical results. There is the natural question as to whether these variables exert

83   significant differences in the prediction of the main flow properties in such region. In this paper, a

84   new two-dimensional (2D) CFD model of the skimming flow in the non-aerated region on stepped

85   spillways is presented. Incompressible turbulent flow is assumed and the free surface is captured

86   by means of Partial- and Complete-VOF methods (Bombardelli et al., 2001; Hirt & Nichols, 1981).

87   The theoretical model is implemented in the open source toolbox *OpenFOAM* and the numerical

88   results are compared against a dataset collected at a facility assembled at the National Laboratory

89   of Civil Engineering (LNEC), in Lisbon, Portugal, available in Matos (1999), Meireles (2004,

90   2011), and Renna (2004). Further, those numerical data are compared with counterparts obtained

91   with the use of the code *FLOW-3D*[®] (Bombardelli et al., 2011). A model sensitivity analysis to

92   different turbulence closures and discretization schemes is performed and discussed. To the best of

93   the Authors' knowledge, such a thorough comparison among different VOF approaches,

94   turbulence models and discretization schemes to determine which of them performs best has not

95   been conducted so far. The flow self-similarity at various locations of the spillway is also assessed

96   by analyzing the flow turbulence properties.

97   It is believed that results of this research provides answers regarding very-important, current

98   discussions on how to model the non-aerated portion of stepped spillways, given the theoretical

99   models included in some codes and packages.

100

2. Experimental data

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103   The experimental facility used for validation of the numerical model presented herein was built

104   at LNEC, in Lisbon, Portugal. The experimental results have been already published elsewhere

105   (e.g., Meireles, 2004, 2011; Bombardelli et al., 2011; Meireles et al., 2012, 2014), so only a brief

106   summary is provided in this section.

107   The facilities consisted of a reservoir, and a smooth crest following the profile of the

108   Waterways Experimental Station (WES). The first steps downstream of the crest had variable size

109   for their edges to fit the WES profile, as depicted in Fig. 1. A tangent point was defined

110   downstream, where the WES profile presented uniform steps. These steps were 3 cm long and 4

111   cm tall, defining a chute slope of 1V:0.75H. The total height of the device, from crest to toe, was

112   2.9 m and had a constant width of 1 m.

113   Measurements were taken using a conductivity probe and a back-flushing Pitot tube held in

114   such a way that measurements could be taken parallel to the spillway pseudo-bottom (see Fig. 2).

115   Even though this work focuses on the non-aerated region of the flow, air concentration

116   measurements helped both to determine the equivalent clear-water depth and to correct

117   differential pressure data in the wavy region. A more thorough discussion on the experimental

118   setup is available in Matos (1999), Meireles (2004, 2011), Renna (2004), Bombardelli et al.

119   (2011), and Meireles et al. (2012, 2014). For the current paper, data presented in Bombardelli et

120   al. (2011), and collected in the framework of Meireles (2004), was considered for the

121   comparative analysis.

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123

3. Theoretical and numerical models

126   *3.1 Flow model*

127   In cases where large domains have to be modeled and no special attention is paid to what

128   occurs at very small time and spatial scales, which generally takes place in most engineering

129   applications, the turbulence averaging of the flow variables in the Navier-Stokes Equations, the so-

130   called Reynolds-Averaged Navier-Stokes (RANS), constitutes the best choice. The RANS

131   Equations [Eqs. (1) and (2) below] are thus solved in this paper. The mass and momentum

132   equations are expressed in vector/tensor notation in the following form, respectively:

133   $$\nabla \cdot \overline{\underline{u}} = 0 \tag{1}$$

134   $$\frac{\partial \overline{\underline{u}}}{\partial t} + \overline{\underline{u}} \cdot \nabla \overline{\underline{u}} = -\frac{1}{\rho} \nabla \overline{p} + \frac{1}{\rho} \nabla \cdot \left(\overline{\underline{\underline{\tau}}} + \underline{\underline{\tau}}^R \right) + \overline{\underline{f_b}} \tag{2}$$

135   where $\overline{\underline{u}}$ is the time-averaged velocity vector, $\overline{p}$ is pressure, ρ indicates the density, t is time, $\underline{\underline{\tau}}$

136   refers to the averaged, deviatoric stress tensor, $\underline{\underline{\tau}}^R$ is the Reynolds stress tensor and $\overline{\underline{f_b}}$ is the

137   gravity force. Surface tension was not included because Weber numbers were always above 110

138   (see Boes & Hager, 2003), thus indicating that this force does not exert a large effect on the flow.

139

140   *3.2 Free surface modeling*

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142   One of the most widely-used methods to capture the position of the free surface is the so-called

143   VOF (Volume of Fluid) method, developed by Hirt and Nichols (1981). This technique is based on

144   three elements: a) the definition of the volume of fluid function (α), which is equal to one when the

145   computational volume is occupied by water, zero when it is air and in between zero and one when

146   the volume is occupied by both air and water; b) the imposition of boundary conditions (i.e.,

147   pressure) at the unknown free surface; and c) the use of an accurate numerical scheme to avoid

148   numerical diffusion of the free surface solution (Bombardelli et al., 2001). Small variants of this

149   method (improvements) are implemented in *FLOW-3D*®, named as TruVOF by the developers

150   (*FLOW-3D*® User Manual, 2016), and those variants have demonstrated their validity in a wide

151   range of hydraulic engineering applications (Bombardelli et al., 2001, 2011; Rodríguez et al.,

152   2004). The VOF method implemented in *FLOW-3D*® has all three ingredients mentioned above. In

153   particular, the implementation of free-surface boundary conditions requires special care to avoid

154   numerical instabilities; further, from the physical point of view, it better reflects the fact that, with

155   the exception of a (thin) boundary layer, water and air generally move independently of each other.

156   In other codes in general, and in *OpenFOAM* in particular, a "Partial" VOF is employed, where

157   both the water and air flows are solved (Bombardelli et al., 2001). This approach presents certain

158   advantages such as accounting for air-water shear stresses; however, it increases the model overall

159   computational cost and may introduce erroneous descriptions in some cases, namely, the

160   simulation of jets coming out of nozzles (Bombardelli et al., 2001).

161   In the TruVOF, the transport of α in the simulated domain is represented by using the

162   following advection equation:

163    $\frac{\partial \alpha}{\partial t} + \nabla \cdot (\overline{\underline{u}}\alpha) = 0$ (3)

164   where $\overline{\underline{u}}$ is the velocity of water. In the Partial VOF method implemented in *OpenFOAM*, the

165   velocity $\overline{\underline{u}}$ is the shared velocity of the two-phase flow. In this Partial VOF method, all variables in

166   each volume, e.g., ξ, are weighted according to the fluid fraction for each fluid A and B:

167    $\xi = \xi_A \alpha + \xi_B (1 - \alpha)$ (4)

168   In the case of *OpenFOAM*, an extra velocity term is added perpendicularly to the water free surface

169   to help to compress it: $\nabla \cdot \left(\overline{\underline{u_c}}\, \alpha[1 - \alpha]\right)$. The term $\alpha[1 - \alpha]$ ensures that the compression velocity

170 only affects those regions where flow fractions are close to 0.5 (Rusche, 2002). The compression

171 velocity term is computed according to a method based on the theory of two-phase flow

172 (Berberovic et al., 2009):

173 $\underline{u}_c = |\underline{u}| \frac{\nabla \alpha}{|\nabla \alpha|}$ (5)

174 where $|\underline{u}|$ is the mixed flow velocity modulus, although in Berberovic et al. (2009), the term $\underline{u}_c$

175 represents the relative velocity between both phases, $\underline{u}_w - \underline{u}_a$.

176 The free surface position is usually defined at the point where $\alpha = 0.5$. More information on free

177 surface modeling can be found in Ubbink (1997), Bombardelli et al. (2001), Rusche (2002) and

178 Berberovic (2010).

179

180 *3.3. Turbulence modeling*

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182 Four different turbulence closures are employed in this work, keeping all the other parameters

183 constant, and their results are analyzed and compared. The four assessed models are the Standard

184 k-ε (Launder & Sharma, 1974), the Realizable k-ε (Shih et al., 1995), the RNG k-ε (Yakhot et al.,

185 1992), and the SST k-ω (Menter, 1993). The models of the k-ε family have proven to yield good

186 results in the modeling of hydraulic structures (Bayon et al., 2016; Bayon & López-Jiménez, 2015;

187 Bombardelli, 2004; Bombardelli et al., 2011; Bradshaw, 1996; Romagnoli et al., 2009; Witt et al.,

188 2015), whereas the SST k-ω model has been successfully applied by the Authors in a study of a

189 hydraulic jump (Bayon & López-Jiménez, 2015).

190 The comparative analysis is conducted exclusively using the RNG k-ε simulations, so that the

191 numerical data obtained with *OpenFOAM* are equivalent to the results obtained by Bombardelli et

192 al. (2011) using *FLOW-3D*®. The RNG k-ε model is a two-equation turbulence model based on the

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193   concept of eddy viscosity ($\nu_t = \frac{\mu_t}{\rho}$), where the two additional variables to compute it are k

194   (turbulent kinetic energy, TKE) and ε (dissipation rate of TKE). The transport of these two

195   variables is modeled according to the following advection-diffusion-reaction (ADR) equations:

196     $\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho k \underline{\overline{u}}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla k\right] + P_k - \rho \varepsilon$ (5)

197     $\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \varepsilon \underline{\overline{u}}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] + (C_{1\varepsilon} - R)\frac{\varepsilon}{k}P_k - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}$ (6)

198     $R = \eta(-\eta/\eta_0 + 1)/(\beta\eta^3 + 1); \quad \eta = Sk/\varepsilon; \quad S = \left(2\overline{S}_{ij}\overline{S}_{ij}\right)^{1/2}$ (7)

199   where P_k is the production of TKE and $\overline{S}_{ij}$ is the strain-rate tensor. The formulation constants are

200     $\sigma_k = 0.7194, \sigma_\varepsilon = 0.7194, c_{1\varepsilon} = 1.42, c_{2\varepsilon} = 1.68, C_\mu = 0.0845, \eta_0 = 4.38,$ and $\beta = 0.012.$

201   The eddy viscosity is computed as $\nu_t = C_\mu\frac{k^2}{\varepsilon}.$

202

203   *3.4. Boundary conditions*

204

205   The boundary conditions imposed to the model are as follows. At the inlet, a constant-depth

206   subcritical flow is followed by a stretch of reservoir of 1.2m in length (measured from the

207   boundary to the crest of the spillway). This buffer zone is long enough according to the Authors'

208   experience (Bombardelli et al., 2011; Toro et al., 2016). Downstream of the spillway, an outlet

209   boundary condition is imposed, where the flow leaves the domain in supercritical state. With

210   regards to the turbulence model variables, k, ε and ω, no measurements are available at the

211   reservoir entrance. Therefore, a Dirichlet boundary condition is set to a low value for the actual

212   profiles to develop along the reservoir buffer stretch.

213   The upper boundary condition of the model is atmospheric and so the flow can freely enter or

214   exit the domain through it; all variables are set to a null von Neumann boundary condition, except

215   for pressure, which is set to atmospheric. A smooth no-slip boundary condition is applied to the

216   solid contours of the model (the roughness of the methacrylate of the experimental device is

217   negligible). Additionally, wall functions are imposed to the solid boundaries in the k-ε family

218   models. The values of y^+ throughout the entire chute were such that the first node was located

219   outside of the viscous sub-layer, thus ensuring that the wall function was operating as intended.

220   Therefore, all mesh elements in contact with solid boundaries have a y^+ coordinate at the

221   logarithmic layer, i.e. $y^+ \in [30,100]$ (Ferziger & Peric, 2012; Schlichting & Gersten, 2000). The

222   y^+ variable is defined as $y^+ = y\frac{u_\tau}{\upsilon}$, where y is the distance of the center of the first volume to the

223   wall, u_τ is the shear velocity, and υ is the kinematic viscosity. On the other hand, since the SST k-

224   ω is a low-Reynolds model, a mesh refinement is required for all mesh volumes in contact with

225   solid boundaries, so that the first volume is in the viscous sub-layer.

226

227   *3.5. Numerical schemes*

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229   The numerical solution of the equations presented above was developed via the finite-volume

230   method (FVM), and implemented in the code *OpenFOAM* (*OpenFOAM* User Guide, 2011). In

231   *OpenFOAM*, the numerical integration is conducted using the PIMPLE algorithm, a combination

232   of two widely used algorithms: PISO (Issa, 1985) and SIMPLE (Patankar & Spalding, 1972).

233   In the present work, three different discretization schemes are used to approximate the

234   advection terms: a) a first-order upwind method; b) the second-order limited Van Leer (1977)

235   method; and c) a second-order limited central difference method. A sensitivity analysis to the

236   numerical discretization scheme is conducted along with the rest of model parameters.

237 Time derivatives are discretized using a second-order backward discretization scheme. The

238 diffusive terms of the equations are discretized using a second-order accurate Gauss linear

239 corrected scheme in all cases.

240

241 **4. Model implementation**

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243 *4.1. Geometry and mesh*

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245 A structured mesh formed by rectangular elements of 4/3 aspect ratio was employed, as was

246 done in Bombardelli et al. (2011). The mesh employed in the SST k-ω simulations required

247 additional refinement in the near-wall region to ensure that y^+ remains within the viscous sub-

248 layer. To this end, 10 extra layers of total thickness equal to 1/3 of the normal element size and a

249 growth ratio of 1.175 were added to the elements adjacent to the spillway steps.

250 In order to fit the mesh to the modeled geometry, the OpenFOAM model uses the tool

251 *snappyHexMesh*; its use in similar applications has yielded good results (Sweeney, 2014; Toro et

252 al., 2016). The *FLOW-3D*® code uses the porosity-based FAVOR method to define solid objects,

253 which, if correctly used, yields accurate results (Bombardelli et al., 2011; Carvalho et al., 2008).

254 To obtain mesh-independent results, 5 different mesh sizes were used and the grid convergence

255 index (GCI) methodology proposed by Roache (2009) was employed. This procedure, based on the

256 Richardson Extrapolation, is discussed and exemplified in Celik et al. (2008). The grid refinement

257 degree between consecutive sizes is $r = \sqrt{2}$, thus being the global refinement degree $r_g = 4.0$,

258 above the 1.3 minimum value proposed by Celik et al. (2008). Mesh refinement is conducted

259 systematically using $h = \sqrt{\Delta x \Delta y}$ as mesh size indicator. The characteristics of the tested meshes

260 are summarized in Table 1. Water depths (d) at 6 different locations are used as indicator variables

261 to compute the residual error among successive mesh sizes. Fig. 3 shows mesh number 5 in the

262 crest zone as an example.

263

Mesh number	Horiz. size (Δx) (mm)	Vert. size (Δy) (mm)	Aspect ratio (V/H)	$h = \sqrt{\Delta x \Delta y}$ (mm)
1	1.06	1.41	4/3	1.22
2	1.50	2.00	4/3	1.73
3	2.12	2.83	4/3	2.45
4	3.00	4.00	4/3	3.46
5	4.24	5.66	4/3	4.90

264 ***Table 1.*** *Characteristics of the meshes tested in the convergence analysis.*

265

266 Simulations were compared against the LNEC experimental data for a discharge of 0.18m^3/s

267 (specific discharge of 0.18m^2/s). These simulations were run varying only one parameter from one

268 simulation to another in order to capture the effect of that specific parameter.

269

270 **5. Analysis of results**

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272 *5.1. Mesh convergence*

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274 The mesh-convergence analysis was conducted using the results obtained with a first-order

275 discretization scheme, as this was the setup used in Bombardelli et al. (2011). In Fig. 4, a

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276   comparison of water free surface profiles for $\alpha = 0.5$ obtained with different mesh sizes is shown.

277   The apparent order reaches a value of $p_{k-\varepsilon} = 0.927$ and $p_{k-\omega} = 0.924$ for the RNG k-ε model

278   and the SST k-ω model, respectively, both close to the model formal order in mesh number 2

279   ($h = 1.73mm$), which indicates that the asymptotic range has been reached. The analysis of these

280   meshes indicates that the average approximate relative error in the indicator variables was

281    $e_{a\,(k-\varepsilon)} = 3.7\%$ and $e_{a\,(k-\omega)} = 3.4\%$. The grid convergence index was $GCI_{k-\varepsilon} = 4.9\%$ and

282    $GCI_{k-\omega} = 4.4\%$, respectively, revealing that in both cases numerical uncertainty remains within

283   acceptable ranges as used in the literature. None of the indicator parameters of the mesh

284   convergence analysis shows improvement at sizes below the size of mesh number 2 ($h =$

285    $1.73mm$). All subsequent analyses are conducted on results employing the mesh of $h = 1.73mm$.

286   Clearly, both codes, *OpenFOAM* and *FLOW-3D*®, respond differently to mesh size reduction.

287

288   *5.2. Sensitivity analysis*

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290   This analysis was exclusively conducted using *OpenFOAM* results, as *FLOW-3D*® results have

291   already been analyzed in Bombardelli et al. (2011).

292   As expected, second-order methods yield more accurate results than their first-order

293   counterparts; however, all schemes tend to underestimate mean flow velocities with a consistent

294   overestimation of flow depths. Differences between first- and second-order methods are small

295   when predicting these variables (4%), but they reach larger values (not shown herein) when

296   predicting maximum TKE on step edges. The differences in the model outcome are small among

297   different second-order discretization schemes (Fig. 5): both limited central-difference and limited

298   Van Leer discretization schemes yield differences in estimations below 4% compared to

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299 experimental data for all the analyzed variables. Nevertheless, the limited central-difference

300 scheme seems to systematically achieve accuracies between 5% and 10% higher employing

301 approximately 30% smaller computational times than the Van Leer scheme.

302   With regard to turbulence models, it is shown in Fig. 6 that the RNG k-ε, the Standard k-ε and

303 the Realizable k-ε models yield virtually the same results (differences are on average below 1%),

304 as expected. On average terms, a slightly better performance can be attributed to the RNG k-ε

305 model in the prediction of certain variables, such as water depths or the profiles within the

306 boundary layer, but this difference is not rather small. As depicted in Fig. 6, the SST k-ω model

307 tends to overestimate water depths (4%) with a consistent underestimation of velocities slightly

308 above the SST k-ε (2% overestimation of water depths). It can also be observed how the latter

309 model yields more developed velocity profiles than the SST k-ω models, although these

310 differences become insignificant when predicting velocity profiles within step cavities.

311

312 *5.3. Discussion of approaches and self-similarity analysis*

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314   The flow depth throughout the stepped spillway is very well predicted by all approaches (see

315 Fig. 7). The first reach located over the smooth region near the spillway crest is reproduced with a

316 root mean square error (RMSE) below 1%. In the last steps, all approaches seem to overestimate

317 the experimental results, although results with TruVOF are slightly closer to the experimental data.

318 The RMSE in the water profile estimation for the TruVOF method is 4.2%, slightly below the

319 6.2% attained by the Partial VOF.

320   With regards to velocity profiles, the formation of a boundary layer is accurately captured by

321 both methodologies (see Fig. 8), although rather significant differences can be observed among

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322 them. For example, the Partial VOF predicts more developed boundary layers than the TruVOF.

323 Both approaches tend to slightly underestimate the velocity values, although the Partial VOF

324 achieves a smaller difference with the experimental data than the TruVOF method. This may be

325 due, among other causes, to the fact that the TruVOF does not account for free-surface tangential

326 stresses. In both cases, this velocity underestimation is consistent with the overestimation of flow

327 depths discussed above.

328 Compared to the velocity profiles obtained through a very recent three-dimensional (3D)

329 detached eddy simulation (Toro et al., 2017), the velocity profiles obtained in this work are very

330 close to those of 3D simulations, confirming that the 2D approach can give useful results for most

331 engineering purposes, and 3D results can be reserved for research.

332 In Fig. 9, the evolution of flow depths and boundary-layer development for both Partial VOF

333 and TruVOF methods is presented. By extrapolating their trending curves, the approximate

334 location of the inception point, i.e., where flow aeration starts, can be estimated. According to this

335 extrapolation, Partial VOF predicted a distance to the inception point of 1.66m, whereas the

336 TruVOF estimated 1.87m. Compared to the experimentally observed distance to the inception

337 point, Partial VOF and TruVOF overestimated this variable by 14% and 30%, respectively. It bears

338 emphasis that the experimental data have uncertainties on its own given the difficulty of

339 determining the precise location of the inception point due to unsteadiness.

340 The experimental results and the inception point location computed according to Chanson

341 (2002) are also included in Fig. 9. Compared to this dataset, the results of Partial VOF and TruVOF

342 differ with experiments in 2% and 7%, respectively, which is indeed accurate enough for

343 engineering purposes. A recent experimental work (Zhang & Chanson, 2016a) states that the

344 inception point occurs where the boundary layer thickness reaches 80% of the water depth. Using

345   this criterion, the Partial VOF and TruVOF estimate distances to the inception point of 1.33m and

346   1.28m, respectively. Compared to the experimental data, the models underestimated this variable

347   by 8% and 12%, respectively. Toro et al. (2017) have very recently shown that cylindrical vortex

348   tubes develop and evolve with space throughout the boundary layer growth, being responsible for

349   the perturbations of the free surface which lead to air entrainment. The complex nature of these

350   tubes can help understand the typical unsteadiness observed in the laboratory experiments and the

351   difficulty of predicting the location of the inception point with accuracy.

352   As discussed above, a certain trend to yield more developed velocity profiles near the spillway

353   crest is observed from the computations using Partial VOF, resulting in a clear overestimation of

354   the boundary-layer thickness within this region ($L < 0.75m$).

355   Meireles (2011) and Toro et al. (2016) proposed and corroborated self-similarity of turbulence

356   statistics in stepped spillways, an unprecedented result. Similarly, Felder and Chanson (2011)

357   discussed self-similarity of the integral time scales in terms of similar trends in the flow

358   distributions along the cavity. However, there was no clear description of the self-similarity in the

359   flow velocity within the cavity, as no negative velocities were recorded in the recirculation region.

360   Previously, in Gonzalez and Chanson (2004), similar trends of the flow velocity within the cavity

361   were presented; in that study, non-dimensional velocities were obtained by using the velocity at

362   which half of the freestream velocity is reached.

363   In the case presented herein, the results show the occurrence of a certain pattern in the velocity

364   and TKE distributions throughout the spillway (see Fig. 10). Using a suitable normalization, most

365   of flow variables present self-similar behavior throughout the spillway. This fact was investigated

366   by using exclusively *OpenFOAM* data and the results indicate approximate flow self-similarity.

367   Fig. 11 shows the normalized profiles of velocity, TKE, dissipation rate and pressure at

368   different step edges compared with the results reported in previous works for the velocities. These

369   profiles show an important degree of overlapping. Additionally, it was observed that the highest

370   pressures always occur close to the pseudo-bottom at approximately 0.32cm upstream of the step

371   edges (cf. also with Toro et al., 2016).

372   A self-similar behavior can also be observed in the step cavities, as depicted in Fig. 12,

373   although the differences in the velocity profiles discussed above are not apparent. The velocity

374   profiles predicted by the model in the recirculation zone attain an accuracy of 93.3%, compared to

375   data by Amador et al. (2006). The same authors state that the maximum recirculation velocity is

376   15% of U_{max}, which is confirmed by the results presented herein. With regards to pressure

377   profiles, it can be observed that this variable drastically drops below the hydrostatic profile in the

378   recirculation region, even attaining negative values, as reported in Toro et al. (2016). It can also be

379   observed that this pressure drop reaches higher values as the distance to the crest increases.

380   Concerning the TKE and dissipation rate of TKE profiles, a peak can be neatly identified near

381   the pseudo-bottom, thus corroborating that the flow in the pseudo-bottom vicinity is responsible for

382   the highest dissipation rates of TKE (Toro et al., 2016, 2017). It was also observed that the

383   dissipation rate profiles perfectly reproduce the shape of the integral turbulent length scale profiles

384   reported in Amador et al. (2006). Toro et al. (2016, 2017) additionally found in the 3D detached

385   eddy simulations that the pseudo-bottom is where vorticity and production of TKE both present a

386   peak, highlighting the tremendous importance of such plane in shedding the tubular structures

387   which are responsible for the deformation of the free surface and, thus, for the air entrainment.

388

389   **6. Final remarks and conclusions**

390   A numerical model, able to reproduce the behavior of the non-aerated region of the flow in

391   stepped spillways, has been implemented using *OpenFOAM*. For its validation, experimental

392   data previously collected at LNEC were used. After conducting a mesh-convergence analysis,

393   the sensitivity to turbulence model, treatment of the free surface and numerical discretization

394   scheme was assessed.

395   Numerical results indicate that the use of a Partial VOF instead of the TruVOF does not

396   affect decisively the predictions of flow velocities and turbulence statistics, although more

397   accurate results can be attributed to the Partial VOF. This result is especially important given the

398   imposition of boundary conditions at the free surface in the TruVOF, which makes it the most

399   cost-effective choice in terms of computational expenses in cases where no strong air-water

400   interaction is expected.

401   The results obtained with several RANS k-ε turbulence models indicate that their predictions

402   of virtually all variables differ less than 1%. The RNG k-ε model performs marginally better,

403   whereas the Standard k-ε and the Realizable k-ε yield virtually the same results. The SST k-ω

404   model, in turn, overestimates the water depths by 4%, with a consistent underprediction of

405   velocities. Differences are more important than those obtained with the models of the k-ε family

406   while solving the flow within the viscous sub-layer. This suggests, at least for this particular case,

407   the benefit of using the RNG k-ε for its smaller computational cost and higher accuracy

408   compared to the SST k-ω.

409   The model sensitivity to different numerical discretization schemes shows that the limited

410   central-difference scheme performs slightly better and at smaller computational costs than the

411   limited Van Leer model, although both second-order schemes yield similar results for velocities

412 and water depths. Its larger accuracy and low computational cost compared to other second-order

413 schemes makes the limited central-difference the most suitable scheme for cases of this nature.

414   Finally, the approximate self-similar behavior of turbulence quantities for the flow on

415 stepped spillways, proposed by our research group elsewhere, was further confirmed in this

416 paper. It was also found that the pressure near step edges raises above the hydrostatic profile,

417 being the maximum value slightly upstream of the step edge. Additionally, special attention is

418 placed on the flow self-similarity within the step cavities, finding that the model presented herein

419 correctly reproduces the data available in the literature for recirculation velocities.

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426

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551

552

553 **Figures**

554

555   **Figure 1.** Geometry of the case study and details of the spillway crest zone. Adapted from

556 Bayon et al. (2015).

557

558   **Figure 2.** Experimental stepped spillway facility at the LNEC, used for experimental

559 validation (Matos, 1999; Meireles, 2004, 2011; Renna, 2004).

560

561   **Figure 3.** Detail of mesh of the spillway crest zone.

562

563   **Figure 4.** Water free surface profiles (left) and velocity profiles (right) at $L = 1.04m$ (step

564 23) as a function of mesh element minimum size (Δx), with a first-order upwind scheme, Partial

565 VOF and the RNG $k - \varepsilon$ model, compared against experimental data. Unfilled symbols indicate

566 measurements affected by fluctuations either of the free surface or the inception point position.

567

568   **Figure 5.** Numerical results using RNG $k - \varepsilon$ model and diverse discretization schemes,

569 with a converged mesh size of $\Delta x = 1.5mm$. a) Water free surface profiles; b) Velocity profile

570 at step 23 ($L = 1.04m$); c) Velocity profile within the cavity at $L = 1.072m$. For the

571 experimental data, unfilled symbols indicate measurements affected by either the fluctuations of

572 the free surface or the location of the inception point.

573

574   **Figure 6.** Numerical results using a limited central-difference discretization scheme and

575   diverse turbulence models, with a converged mesh size of $\Delta x = 1.5mm$. a) Water free-surface

576   profiles; b) Velocity profile at step 23 ($L = 1.04m$); c) Velocity profile within the cavity at

577      $L = 1.072m$. For the experimental data, unfilled symbols indicate measurements affected by

578   either the fluctuations of the free surface or the location of the inception point.

579

580   **Figure 7.** Water free-surface profile using RNG $k - \varepsilon$ model and first-order upwind

581   discretization scheme and a converged mesh size of $\Delta x = 1.5mm$ according to type of VOF

582   method: Partial VOF (OpenFOAM) and TruVOF (FLOW-3D®).

583

584   **Figure 8.** Velocity profiles using RNG $k - \varepsilon$ model and a first-order upwind discretization

585   scheme and a converged mesh size of $\Delta x = 1.5mm$ according to type of VOF method: Partial

586   VOF (OpenFOAM) and TruVOF (FLOW-3D®).

587

588   **Figure 9.** Distribution of water depths, boundary-layer development and estimated inception

589   point of air entrainment profile using RNG $k - \varepsilon$ model and a first-order upwind discretization

590   scheme and a converged mesh size of $\Delta x = 1.5mm$ according to type of VOF method: Partial

591   VOF (OpenFOAM) and TruVOF (FLOW-3D) with validation using experimental data and

592   literature.

593

594   **Figure 10.** Velocity and TKE fields throughout the spillway obtained with OpenFOAM

595   using a converged mesh ($\Delta x = 1.5mm$), an upwind first-order discretization scheme and the

596   RNG $k - \varepsilon$ model.

597

598   **Figure 11.** Profiles of normalized velocity, turbulent kinetic energy (TKE), dissipation rate

599   of TKE and pressure at different step edges using RNG $k - \varepsilon$ model and a first-order upwind

600   discretization scheme and a converged mesh size of $\Delta x = 1.5mm$. In the pressure plot, unfilled

601   symbols correspond to pressure profiles $0.32\ cm$ upstream of step edges, where maximum

602   pressure occurs, and p_0 is the hydrostatic pressure at the pseudo-bottom.

603

604   **Figure 12.** Profiles of normalized velocity, turbulent kinetic energy (TKE), dissipation rate

605   of TKE and pressure at different step gaps using RNG $k - \varepsilon$ model and a first-order upwind

606   discretization scheme and a converged mesh size of $\Delta x = 1.5mm$.

607

608

609

610

Local Coordinate System (LCS)

WES spillway:
$$x^{1.85} = 0.4027^{0.85}y$$
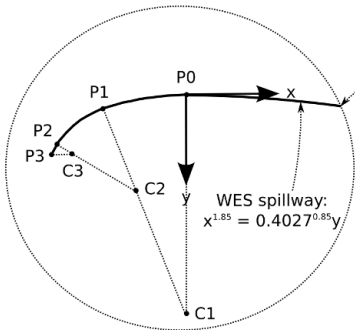
Point	x (m)	y (m)
P0	0.000	0.000
P1	-0.035	0.006
P2	-0.056	0.023
P3	-0.057	0.027

			Arc	radius (m)
C1	0.000	0.101	C1	0.101
C2	-0.021	0.044	C2	0.040
C3	-0.049	0.027	C3	0.008

Global Coordinate System (GCS)

crest
(L = 0.000m)

boundary layer development

non-aerated region

WES spillway

pseudo-bottom

tangent point
(L = 0.440m)

constant slope
(1V : 0.75H)

inception point
(L = L)

aerated region
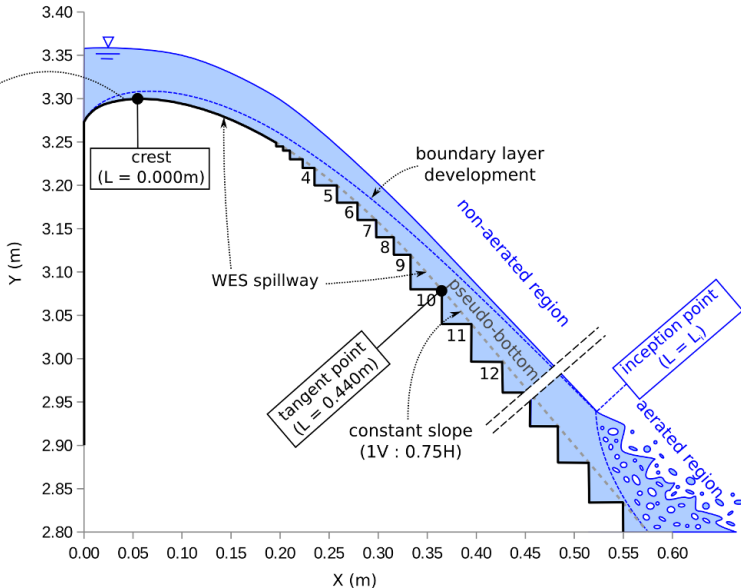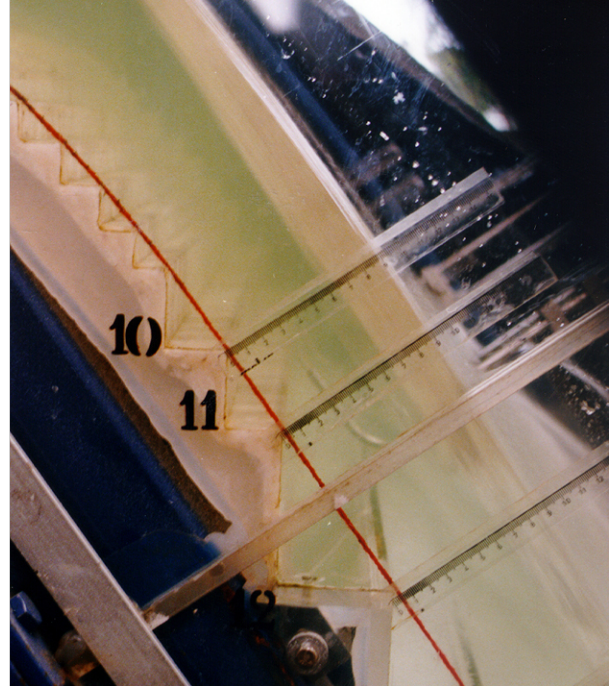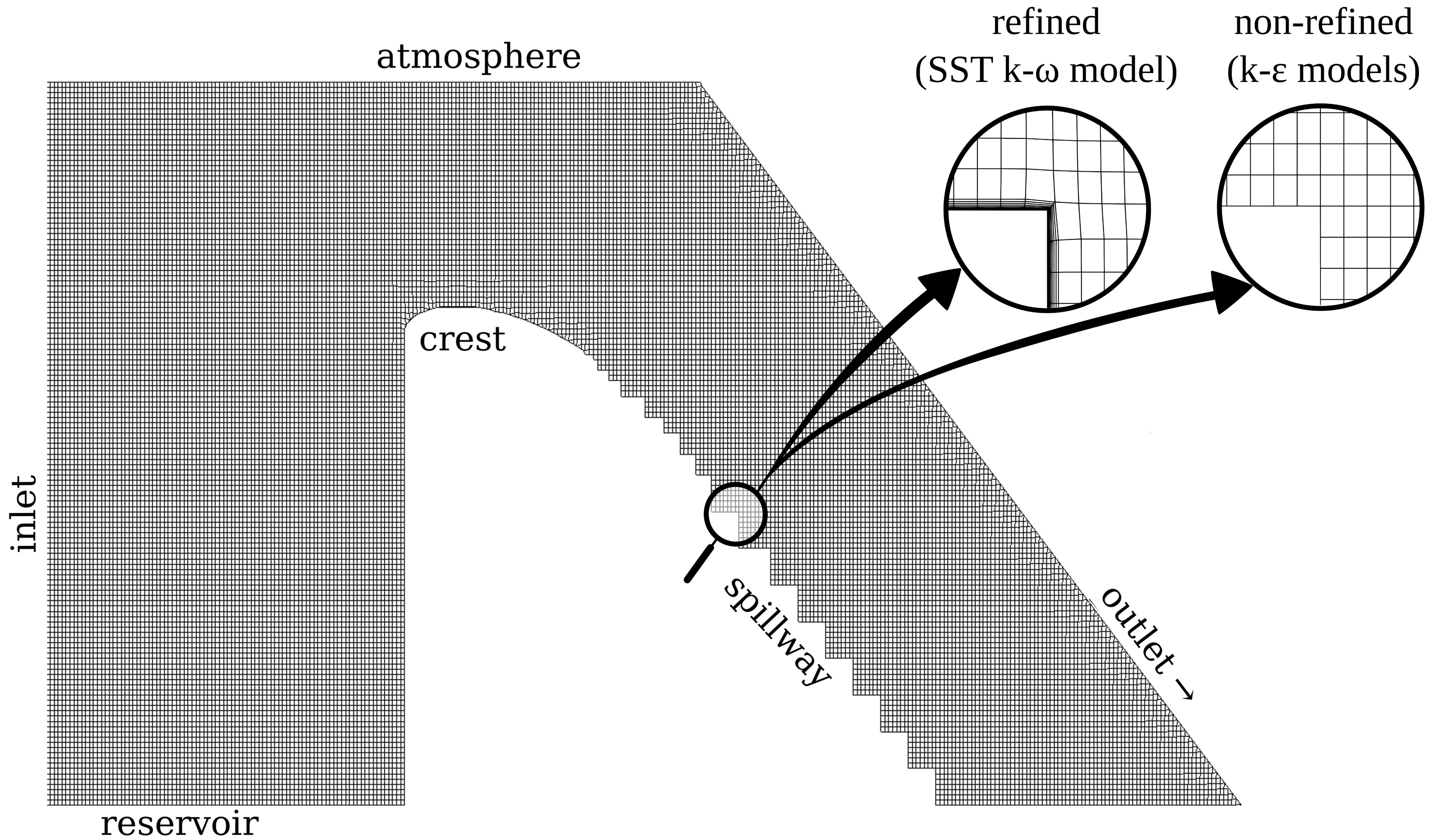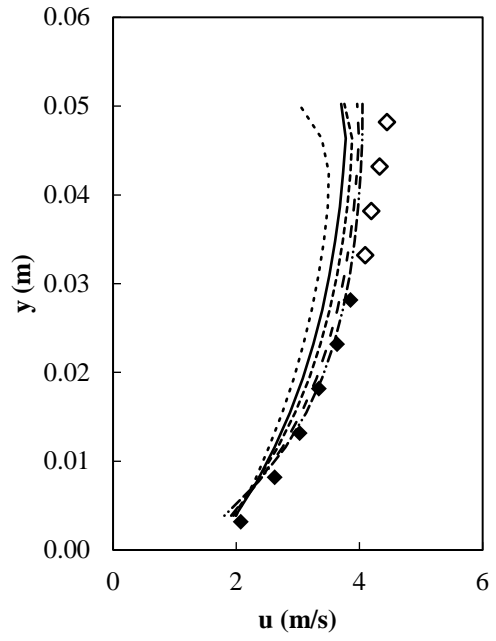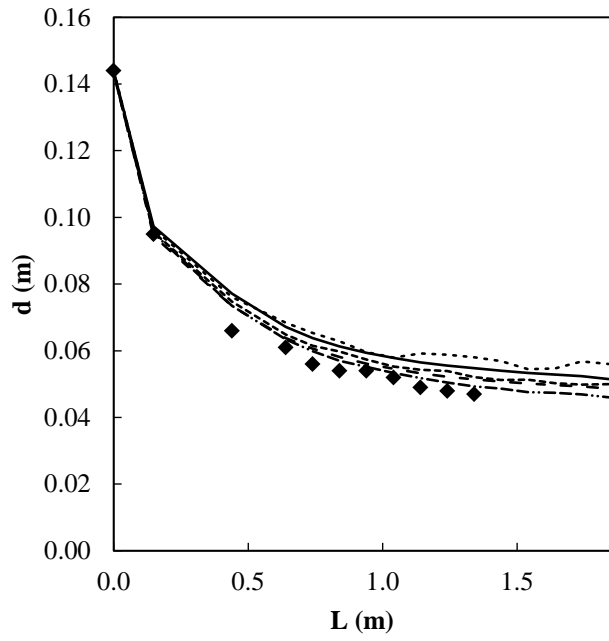
--·····-- Δx=1.1mm - - - Δx=1.5mm ------- Δx=2.1mm ———— Δx=3.0mm ······· Δx=4.2mm ◆ Experimental

d (m) — **L (m)**

y (m) — **u (m/s)**

y (m) — **u (m/s)**
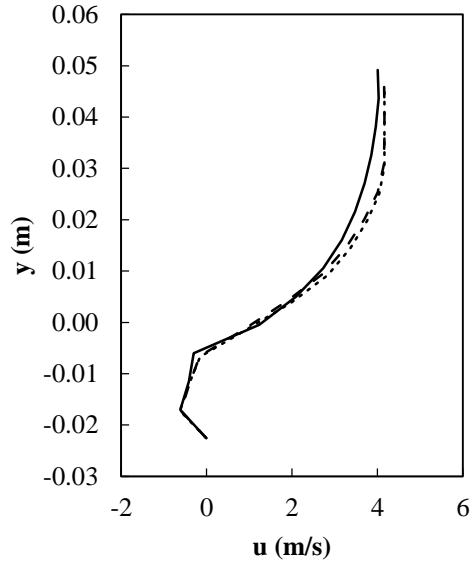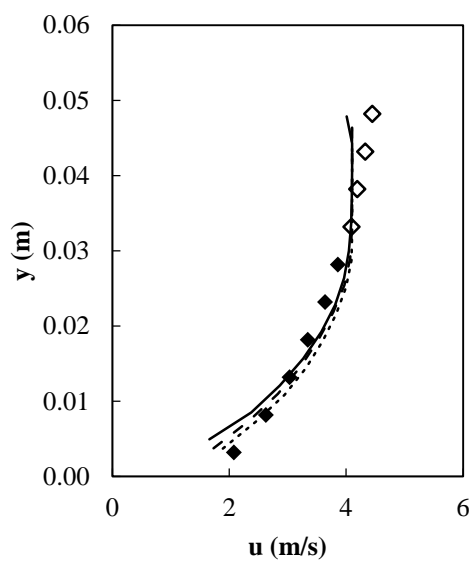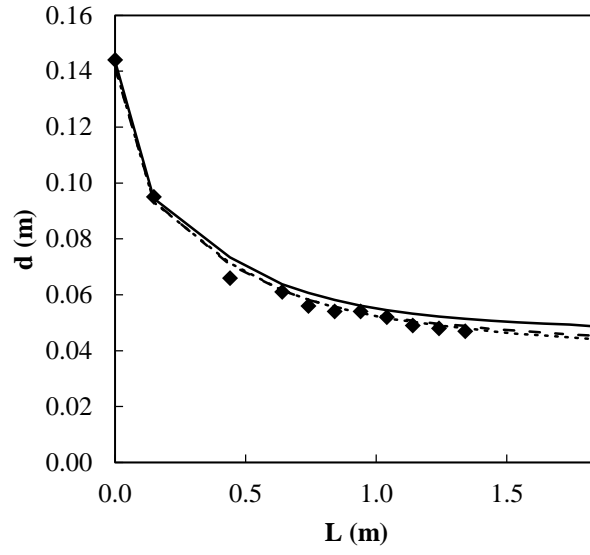
——— 1st order upwind   ⋯⋯⋯Limited Linear   – – Van Leer   ◆ Experimental

d (m)

L (m)

y (m)

u (m/s)

y (m)

u (m/s)

- - - Realizable k-ε ——— RNG k-ε ······· Standard k-ε

— · — · SST k-ω ◆ Experimental

d (m)

0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00

0.0   0.5   1.0   1.5

L (m)

——OpenFOAM   ······FLOW-3D   ◆ Experimental

Step 15 (L = 0.64m)   Step 17 (L = 0.74m)   Step 19 (L = 0.84m)

Step 21 (L = 0.94m)   Step 23 (L = 1.04m)   Step 25 (L = 1.14m)

Step 27 (L = 1.24m)   Step 29 (L = 1.34m)

——OpenFOAM   ······FLOW-3D   ◆ Experimental

Step	15	20	25	30	35
L(m)	0.64	0.89	1.14	1.29	1.64

U (m/s)

Step	15	20	25	30	35
L(m)	0.64	0.89	1.14	1.29	1.64

k (J/kg)
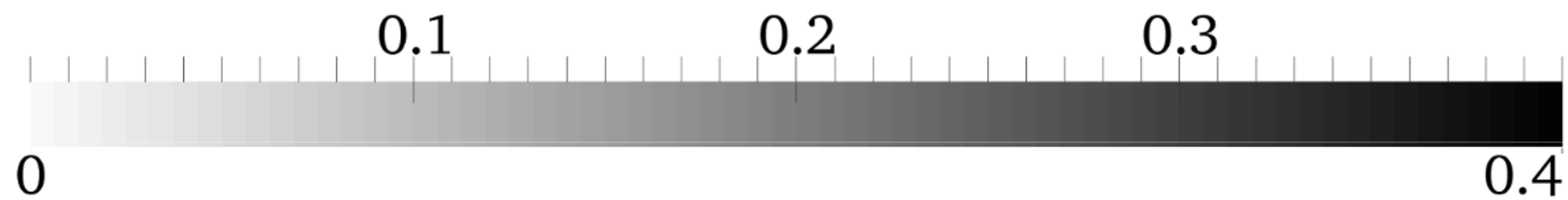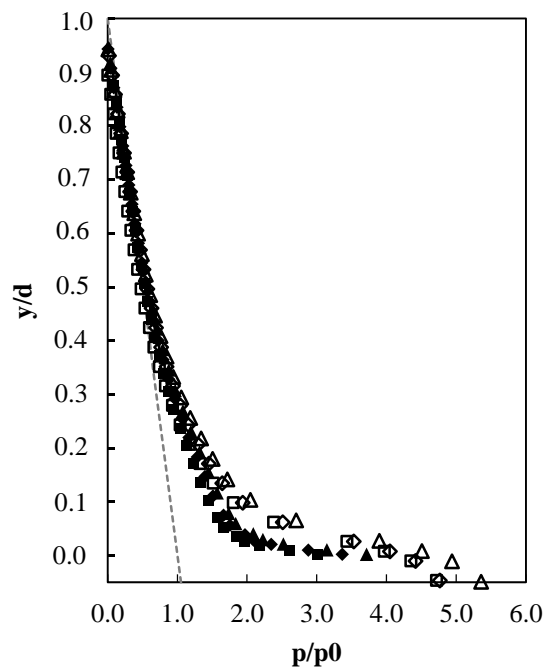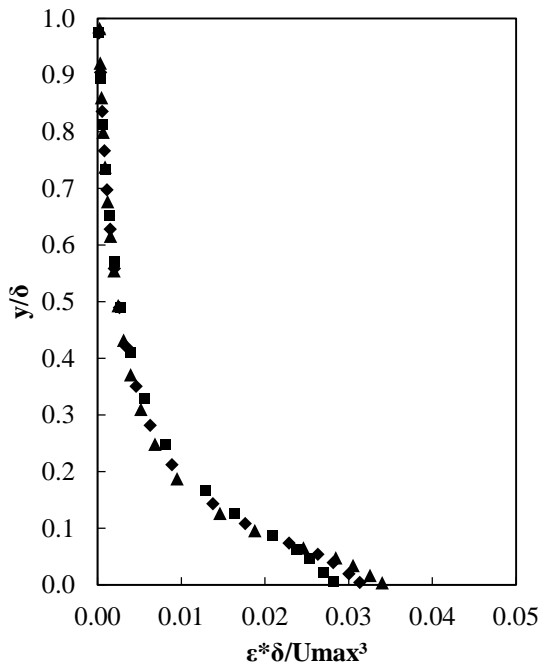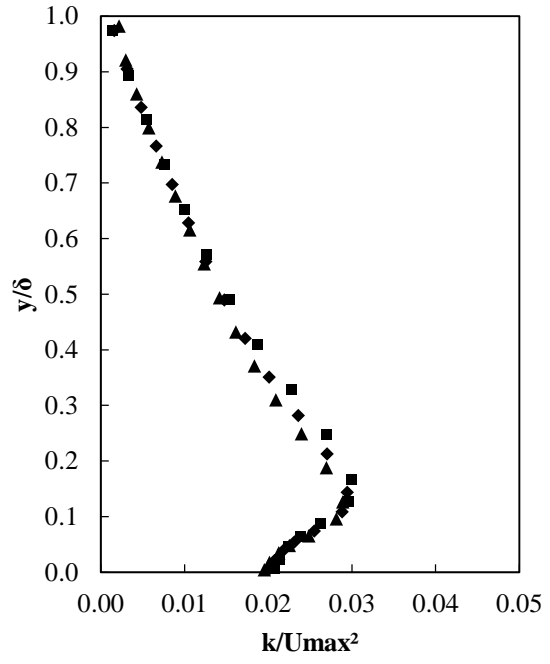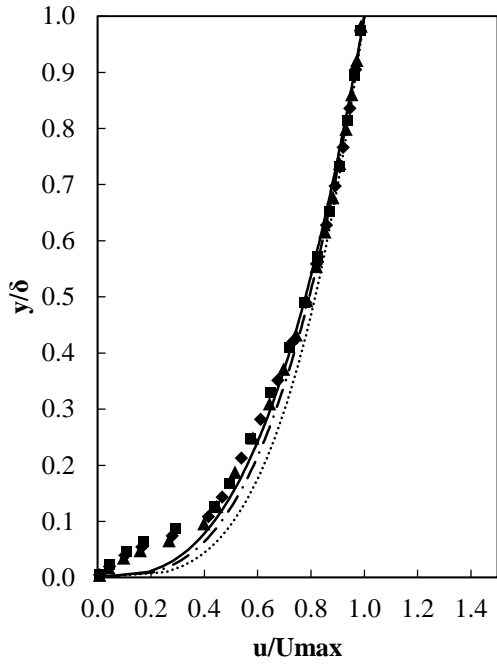
■ Step 19 (L=0.84m)	◆ Step 23 (L=1.04m)	▲ Step 27 (L=1.24m)
⋯⋯ Meireles et al. (2012)	— · — Amador et al. (2006)	- - - - Hydrostatic profile
——— CFD		
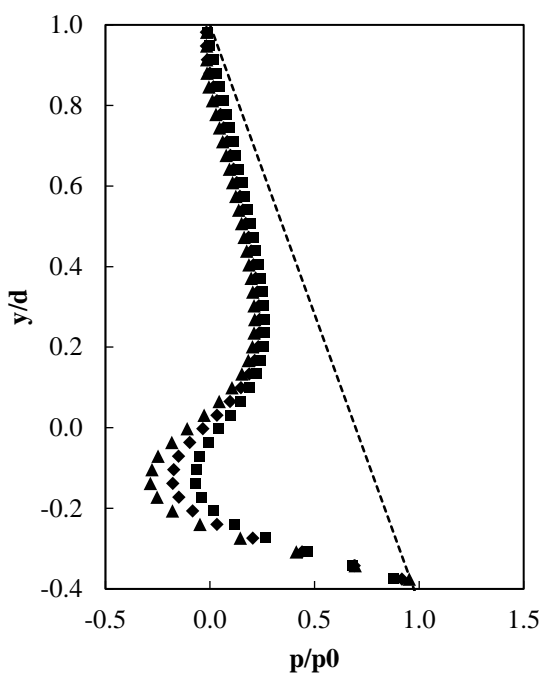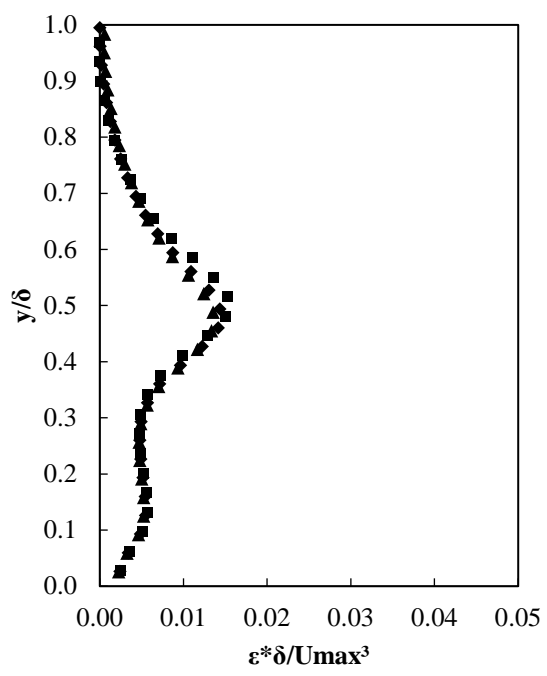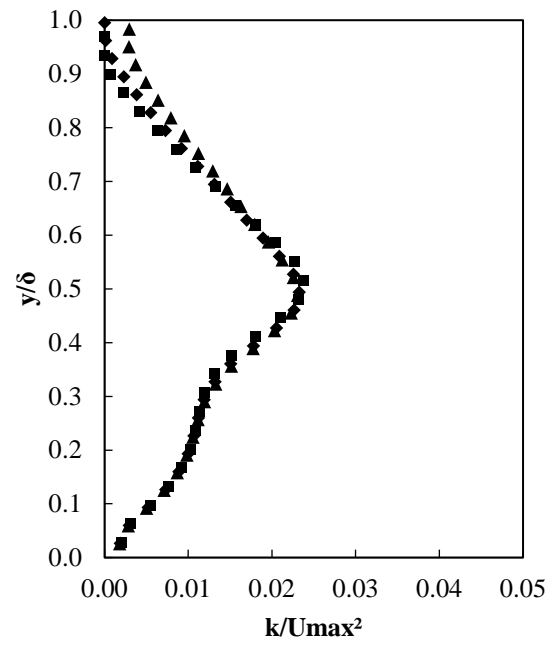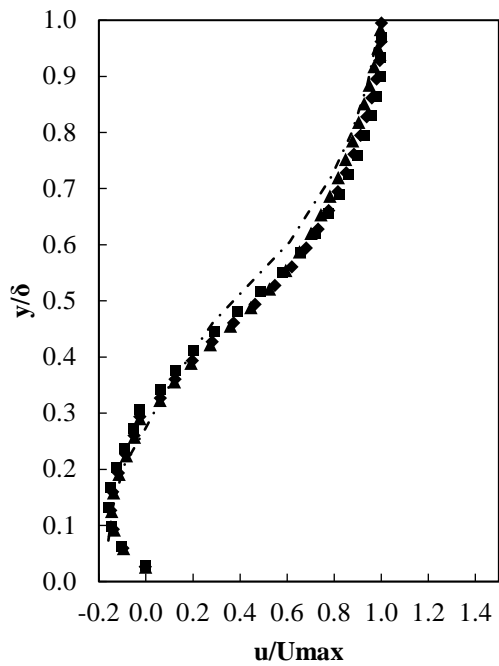
Symbol	Legend
■	L=0.872m
◆	L=1.072m
▲	L=1.272m
- - - -	Hydrostatic
- · - · -	Amador et al. (2006)