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A MULTILEVEL APPROACH IN THE NUMERICAL MODELLING OF A FLOW ACCELERATED CORROSION PHENOMENON

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Abstract. *Flow Accelerated Corrosion (FAC) is a spontaneous and undesirable mass transfer phenomenon that occurs in several industries. Due to the great cost associated with the corrosion phenomenon in fluid dynamic systems, the application of different CFD techniques is necessary to obtain methods that enable the estimation of the corrosion rate with accuracy and low computational cost. In the present study, the application of a multilevel method in a sudden expansion pipe flow was evaluated to analyze the corrosion phenomenon in these fluid dynamic systems, with high accuracy and shorter computational times. For the analysis of the multilevel approach, the mass transfer phenomena and the fluid dynamics were solved considering the continuity, Navier-Stokes, and passive scalar transport equations. As for the turbulence closure modeling, the URANS model applied is the Low Reynolds Number k-ε model of Abe-Kondoh-Nagano (AKN). The advantage in applying the multilevel method for this case scenario can be explained by the high Schmidt number of the flow. With the high Schmidt number (Sc = 1460), the boundary layer thickness of the mass transfer phenomenon is lower than the momentum boundary layer thickness. With the multilevel method implemented in the MFSim software, it is possible to solve the equations that represent both phenomena in different meshes at the near-wall regions. Numerical-computational simulations were performed with the multilevel method considering the data in the literature. A moderate deviation was observed for this turbulence closure model in the region downstream the reattachment point considering the corrosion rates. Furthermore, small deviations in the corrosion rates were observed upstream of the reattachment point. Regarding the application of the multilevel method, a significant reduction in computational time with high accuracy results were obtained.*

Keywords: *Flow Accelerated Corrosion, Multilevel approach, High Schmidt number*

1. INTRODUCTION

The phenomenon of flow accelerated corrosion (FAC) is present in the oil and gas industry, chemical process industry, and nuclear power plants. In these industries, FAC occurs in complex and turbulent flows and is observed in orifice plates, sudden expansion/contraction, and bend regions. Besides the geometry and shape of the pipes, the pipe material and the fluid properties such as salinity, pH, and temperature also have great influences on the mass transfer phenomenon (Poulson, 2014).

The flow influence under different fluid dynamic conditions was studied experimentally by Sydberger and Lotz (1982). Separation flows were evaluated, and flow conditions with higher Reynolds numbers (*Re*) led to a more critical condition regarding the mass transfer phenomenon. From this study, different computational numerical strategies were evaluated by Nesic, Postlethwaite and Bergstron (1992), and Xiong, Koshizuka and Sakai (2011). Several models for turbulence closure were studied and the model that showed the best accuracy was the one proposed by Abe, Kondoh, and Nagano (1994). Turbulence closure models of RNG *k-ε* and *k-ω* SST also show great accuracy in higher Reynolds number flows in bends as analyzed by Lin and Ferng (2014) and Prasad *et al*. (2018).

The mass transfer phenomena evaluated in these experimental and computational studies have as characteristic a high Schmidt number ($Sc \approx 10^3$). In the mass transfer process analyzed by Nesic, Postlethwaite and Bergstron (1992), it is possible to observe a disparity of the boundary layer thickness lengths required to solve the fluid dynamics and the corrosion phenomenon in parietal regions. Thus, for flows with high Sc, it becomes feasible to implement numerical methodologies that allow solving the balance equations of the fluid-dynamic process and the mass transfer phenomenon on distinct meshes to reduce the computational cost.

In the present study, a multilevel method was used to solve the balance equations of each phenomenon in meshes with different characteristics in the near-wall region. The strategies applied for modeling the corrosion phenomenon with reduced computational costs were defined based on the strategies considered in studies of Ostilla-Monico *et al*. (2015), Kubrak *et al*. (2013), and Panda *et al*. (2019). In each of these studies, a proposal for computational cost reduction was evaluated considering distinct phenomena that have similar characteristics to those observed in FAC systems. Considering the modeling of the phenomena in different meshes, the authors obtained highly accurate results with a significant reduction of computational time.

2. METHODOLOGY

In order to test a robust model for modeling the corrosion phenomena, a multilevel method was evaluated on a sudden expansion flow. The corrosion model, the differential mathematical model, the numerical computational model, and the multilevel approach are detailed in this section.

2.1 Corrosion modelling

The corrosion model defined by Nesic, Postlethwaite and Bergstron (1992), and Keating (1999) were considered to analyze the corrosion phenomenon on the sudden expansion flow. This mass transfer phenomenon is represented by

$$2Fe \rightarrow 2Fe^{++} + 4e^{-}$$
$$O_2 + 2H_2O + 4e^{-} \rightarrow 4OH^{-}. \quad (1)$$

The mass flux from the flow to the wall, *n*, can be defined by

$$n = k_m(C_b - C_w) \quad (2)$$

where C_b is the bulk concentration, C_w is the concentration on the wall, and k_m is the mass transfer coefficient. Considering the oxygen concentration inside the mass transfer boundary layer, the mass transfer coefficient can be expressed by

$$k_m = -D\ \frac{\partial C_0/\partial y|_{y=0}}{C_b} = -\frac{D}{\Delta y}\frac{C_0}{C_b} \quad (3)$$

where D is the diffusivity coefficient, Δy is the distance from the center of the first volume to the wall, and C_0 is the oxygen concentration at that distance. Thus, through numerical simulations the corrosion rate C_r can be calculated by

$$\frac{dC_r}{dt} = 2k_m C_b \quad (4)$$

2.2 Differential mathematical model

The FAC phenomenona on the sudden expansion flow was simulated considering the Unsteady Reynolds Averaged Navier-Stokes (URANS) equations and a concentration balance equation presented in Eq. (5) and Eq. (6), respectively.

$$\rho\frac{\partial U_i}{\partial t} + \rho\frac{\partial}{\partial x_j}\left(U_iU_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\right], \quad (5)$$

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j}\left(U_jC\right) = \left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial^2 C}{\partial x_j \partial x_j}. \quad (6)$$

In Eq. (5), ∂ is the differential operator, ρ is the specific mass of the fluid, U_i is the component *i* of the velocity vector, *t* is the time, x_i is the spatial component in *i* direction, *P* is the pressure, μ is the dynamic viscosity of the fluid and μ_t is the turbulent viscosity. Furthermore, in Eq. (6), C is the concentration, and Sc_t is the turbulent Schmidt number, which was defined 0.9. The turbulence closure model considered is the Low Reynolds Number *k*-ε proposed by Abe, Kondoh and Nagano (1994) (AKN). The turbulent kinetic energy, k [m²/s²], the dissipation rate, ε [m³/s²], and the turbulent viscosity, μ_t, are given by

$$\frac{\partial(\rho k)}{\partial t} + \bar{u}_j \frac{\partial}{\partial x_j}(\rho k) = \frac{\partial}{\partial x_j}\left[(\mu + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial x_j}\right] + \mu_t S^2 - \rho\varepsilon, \tag{7}$$

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \bar{u}_j \frac{\partial}{\partial x_j}(\rho\varepsilon) = \frac{\partial}{\partial x_j}\left[(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial x_j}\right] + C_{\varepsilon 1} f_{\varepsilon 1}\frac{\varepsilon}{k}\mu_t S^2 - \rho C_{\varepsilon 2} f_{\varepsilon 2}\frac{\varepsilon^2}{k}, \tag{8}$$

$$\mu_t = \rho\, f_\mu\, \frac{C_\mu k^2}{\varepsilon}. \tag{9}$$

In Eq. (7) and Eq. (8), $S = \sqrt{S_{ij}S_{ij}}$, in which S_{ij} represents the strain rate tensor components. The model's constants applied to solve the equations are: $c_\mu = 0.09$, $\sigma_k = 1.4, \sigma_\varepsilon = 1.4$, $C_{\varepsilon 2} = 1.5$, and $C_{\varepsilon 2} = 1.9$. In Eq. (8) and (9), the variables $f_{\varepsilon 1}$, $f_{\varepsilon 2}$and f_μ represent the damping functions and are given by

$$f_\mu = \left\{1 - \exp\left(-\frac{R_\varepsilon}{14}\right)\right\}^2 \left[1 + \frac{5}{R_t^{0,75}}\exp\left\{-\left(\frac{R_t}{200}\right)^2\right\}\right], \tag{10}$$

$$f_{\varepsilon 1} = 1, \tag{11}$$

$$f_{\varepsilon 2} = \left\{1 - \exp\left(-\frac{R_\varepsilon}{3{,}1}\right)\right\}^2 \left[1 - 0{,}3\exp\left\{-\left(\frac{R_t}{6{,}5}\right)^2\right\}\right]. \tag{12}$$

where R_ε and R_t are the normalized wall distances, and are obtained by

$$R_t = \frac{\rho k^2}{\mu\varepsilon}, \tag{13}$$

$$R_\varepsilon = \frac{y}{(\nu^3/\varepsilon)^{1/4}}. \tag{14}$$

2.3 Multilevel approach

The modeling of the flow with separation under corrosive effects were performed using the MFSim code, developed at the Fluid Mechanics Laboratory, MFLab, in the Federal University of Uberlândia. One of the characteristics of the MFSim code is the application of the finite volume method to discretize equations. The studies developed from the code are performed using structured block meshes and variable time steps. In other words, the Navier-Stokes equations and the advective-diffusive balance equation of a scalar are solved in MFSim considering a hierarchy of nested Cartesian meshes. As it can be seen in Figure 1, the mesh is characterized by a base physical level, Lbot, which covers the entire computational domain, and a sequence of physical levels that are progressively refined, considering a mesh ratio 2, until the level with the smallest grid spacing, which is called Ltop. It is noteworthy that Figure 1 shows a mesh with characteristics similar to those applied for the numerical modeling of the FAC phenomenon in the MFSim code.

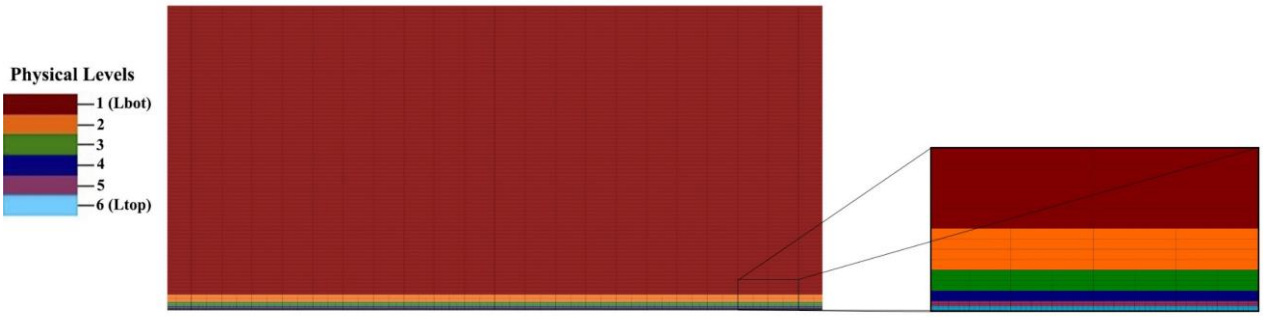

Figure 1. Structured block mesh with six refinement levels.

From Figure 1, it can be seen that for FAC the meshing of the Ltop level is limited only to the parietal regions. In this phenomenon, the grid spacing at the Ltop level is defined by the sub-layer thickness of the mass transfer process that can be obtained by $\delta_{sca} = \delta_{hid}/Sc^{1/3}$ according to Nesic, Postlethwaite and Bergstron (1992). In order to perform the simulation with lower computational cost, it was proposed a method to solve the fluid dynamics phenomena and the mass transfer phenomena on distinct meshes but having the same characteristic at the Lbot level. In order to solve the fluid dynamics equations and the scalar balance equation considering the boundary layer of each phenomenon, the equations referring to fluid dynamics are solved up to an intermediate physical level, l^*, and the scalar balance equation up to Ltop. Thus, it becomes possible to solve the fluid dynamics equations in larger spatial and temporal sizes than the sizes needed to solve equations referring to the corrosion phenomenon.

For the application of the multilevel methodology, it is necessary to interpolate the properties of the flow for solving the scalar advective/diffusive balance equation properly. Considering that the equations are solved at different mesh sizes at near-wall regions, the method detailed by Balsara (2001) was adopted for interpolating the velocity field from the physical level l^* to the upper physical levels. From this interpolation method, it is possible to obtain a conservative velocity field up to the Ltop level so that the scalar balance equations can be solved. The methodology detailed by Balsara (2001) was chosen because it is applicable for meshes with refinement ratios of 2 and because it provides a conservative interpolation process for obtaining the velocity field. In addition, the method can also be applied for high aspect ratio meshes. By implementing this method, it is possible to obtain an extension of the velocity field keeping the divergence-free property for the sequence of physical levels. It is important to mention that the balance equation of k and ε are solved up to the Ltop level, and considers the velocity-interpolated field.

2.4 Computational simulations

In order to validate the proposed methodology and to evaluate the multilevel method, the study performed by Sydberger and Lotz (1982) was considered. Through material experimentation, the authors determined the mass transfer coefficient in pipe flows with contraction/expansion and Schmidt number of 1,460. Among the different expansion and contraction geometries, a sudden expansion flow with a Re = 21,000 (outlet region) was simulated. In addition, the inlet length was defined 20.0 mm and the outlet length was defined 40.0 mm.

A pseudo-2D domain limited to the region after the expansion was considered for the numerical computational modeling. At the inlet, a fully developed flow and a constant oxygen concentration profile were defined. A symmetry condition considering the pipe centerline was set. At the outlet, a Neumann condition was imposed for the properties of the flow and scalar. In parietal regions, k was imposed null and ε was defined by $\varepsilon_w = 2\mu k/(\rho \Delta y^2)$. These boundary conditions were defined in a computational domain with dimensions $0{,}24 \times 0{,}02\ m^2$ $(L \times H)$.

Five simulations were performed to evaluate the multilevel method. The mesh information and other simulation parameters are detailed in Table 1. In addition, a physical time of 4.0 s was defined for the convergence of the flow to the steady-state condition.

Table 1. Numerical simulation data considering the LRN $k-\varepsilon$ AKN model.

Simulation #	1	2	3	4	5
Mesh (Lbot)	120x80	120x80	120x80	120x80	120x80
Physical levels	6	6	6	6	6
Volumes number	763.920	763.920	763.920	763.920	763.920
Δy_{sca} (μm)	3,90625	3,90625	3,90625	3,90625	3,90625
Δy_{vel} (μm)	3,90625	7,8125	15,625	31,25	62,5

In Table 1 it is observed that in the 5 simulations the same mesh was defined to adequately solve the mass transfer phenomenon. In addition, for the fluid dynamics, a different distance from the center of the volume to the wall (Δy_{vel}) was considered to evaluate the efficiency of the multilevel method by analyzing the profile of the mass transfer coefficient and also to evaluate the reduction of computational cost. In these simulations, the time step adopted was determined based on the Courant-Friedrichs-Lewy (1967) criterion, which was calculated based on the properties of the fluid-dynamic mesh.

Regarding the numerical methods in the MFSim, the following were considered: the fractional step method for pressure-velocity coupling; the CUBISTA method for spatial discretization of the advective terms of each balance equation; the multilevel-multigrid method to obtain the solution of the velocities and the scalar; the Petsc to obtain the solution of the pressure. The convergence criterion of 10^{-6} was set to solve the balance equations of the phenomenon. It should be noted that the simulations were performed considering parallel processing, and 12 processes (Intel® Xeon® Silver 4214 CPU 2.20 GHz) were applied.

3. RESULTS AND DISCUSSION

Based on the conditions of the experiments performed by Sydberger and Lotz (1982), the abrupt expansion simulations were evaluated using the MFSim code. The results obtained using the numerical methodology presented were compared to the experimental data. The streamlines of the permanent velocity fields calculated with the LRN k-ε AKN model are shown in Figure 2.

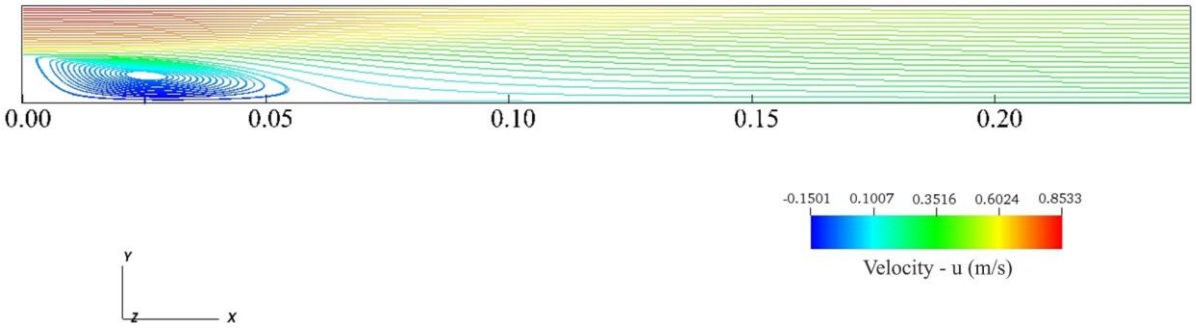

Figure 2. The streamline obtained with the LRN k-ε AKN model.

Figure 2 shows the formation of a recirculation flow near the expansion region. With the velocity profile in the center of the volume closest to the wall, the reattachment lengths were determined for the five simulations. The analysis of the reattachment lengths was necessary to verify that the velocity field obtained through the conservative interpolations would reproduce the velocity field at the wall adequately. For the simulation in which the multilevel method was not applied, the value of the reattachment length, x_r, over the step height, h, was x_r/h = 6.21. For the simulations where multilevel was applied, a maximum deviation of 3.7% was observed in simulation 5. In other words, it can be stated that the interpolated velocity field led to small changes in the fluid dynamic field.

In the simulations where the multilevel method was applied, the parameters k, ε e μ_t are obtained considering the interpolated velocity field. As the turbulent viscosity is an important property in the corrosion phenomenon due to the additional diffusivity effects on the scalar transport phenomenon, it is necessary to perform an evaluation of the multilevel method based on the profile of the k_m in the near-wall region. In Figure 3 is shown the k_m coefficient profiles for the five simulations and the experimental data obtained by Sydberger and Lotz (1982).

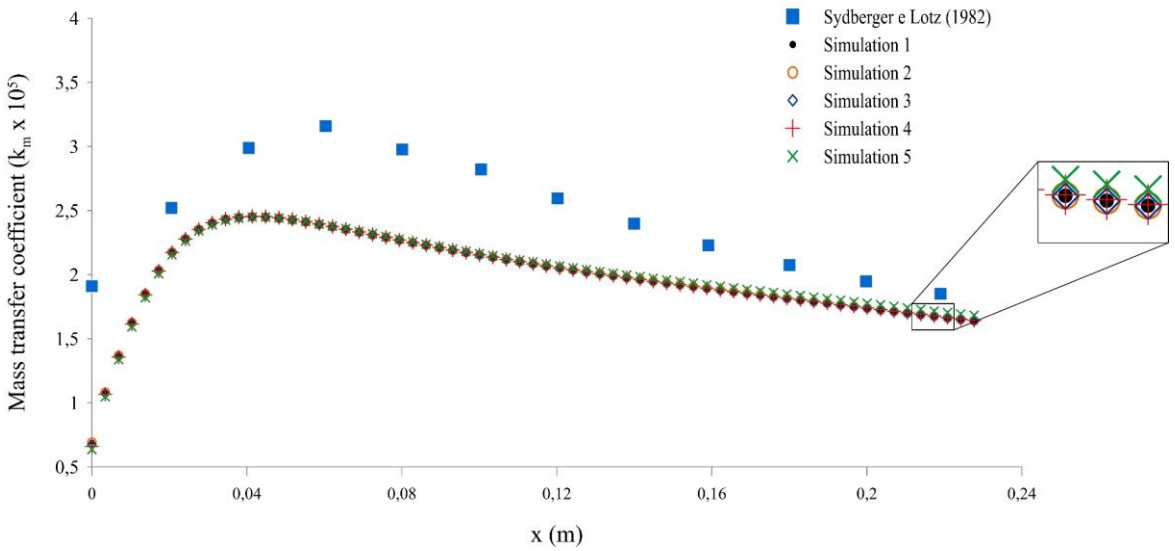

Figure 3. Mass transfer coefficient profile for the sudden expansion flow with Sc =1460.0 and Re = 2.1×10^4.

In Figure 3, the k_m coefficient profiles obtained through the numerical simulations showed moderate deviations for the region near the recirculation zone considering the experimental data. Moreover, at locations further from the reattachment point, the deviation between the experimental and numerical results was smaller. It is important to mention that it was expected to obtain a k_m profile with moderate deviations compared to the experimental data of Sydberger and Lotz (1982). The moderate deviation was expected due to simplifications in the computational domain and also due to

the application of the cartesian coordinate system. In other words, results with smaller deviations would be obtained if the region before the expansion was considered and the applied coordinate system was cylindrical. Regarding the coordinate system, the MFSim software simulates flows only in the cartesian coordinate system. Nevertheless, it is important to emphasize that the main objective of the present study is to analyze the multilevel method, and the result obtained in simulation 1 is already adequate for the analysis of this multilevel approach.

Considering the simplifications, the analysis of the multiscale method was performed comparing the results from simulations 2 to 5 with simulation 1. From Figure 3, it can be affirmed that the results obtained in simulations 2-4 showed a negligent deviation considering the k_m profile in simulation 1. Furthermore, in Simulation 5 a small deviation is observed after the reattachment point. Therefore, it was observed in Figure 3 that solving the mass transfer phenomenon in the near-wall region with an interpolated fluid dynamics field resulted in small deviations. The computational cost of the simulations is detailed in Table 2.

Table 2. Computational cost evaluation with the multilevel approach

Simulation #	1	2	3	4	5
Iterations	512008	256008	128008	64008	32008
CPU time- velu (s)	0,0165	0,0115	0,0087	0,0080	0,0068
CPU time - velv (s)	0,0188	0,0125	0,0094	0,0076	0,0076
CPU time - pressure (s)	0,3960	0,208	0,0121	0,0080	0,0596
CPU time - scalar (s)	0,0612	0,0623	0,0667	0,0787	0,10
CPU time - k (s)	0,0608	0,0598	0,0620	0,118	0,134
CPU time - ε (s)	0,1220	0,121	0,119	0,177	0,238
CPU time - interpolation (s)	0,0000	7,04e-04	0,00108	0,00134	0,00138
CPU time per iteration (s)	0,863	0,644	0,546	0,625	0,696
Total simulation time (hours)	120,26	45,82	19,40	11,10	6,19

From the data in Table 2, one can see a gradual reduction of the total simulation time as the fluid dynamics equations are solved on a coarser mesh. The main parameters that contributed to the gain in numerical-computational efficiency were the shorter computational time to solve the pressure, velocities, and the application of a restricted time step to the fluid dynamics. In addition, it was observed that the time required for the conservative interpolation of the velocity field at each iteration has no significant influence on the computational cost. The highest efficiency gain without considerable deviations in the k_m profile was observed in simulation 5, in which there was a reduction in computational time of approximately 19.4 times.

4. CONCLUSIONS

The flow accelerated corrosion phenomenon was numerically simulated considering the turbulence model proposed by Abe, Kondoh, and Nagano (1994). Consistent results were obtained in the MFSim software based on the experimental data and the evaluated methodology. In addition, the multilevel method was proved robust because it allows the modeling of the corrosion phenomenon with a lower computational cost and high accuracy. The highest computational time reduction observed was 19.4 times with the LRN k-e AKN model. In the simulations, it was possible to solve the corrosion phenomenon accurately considering a ratio of 16, between the fluid dynamics mesh length and the corrosion mesh length in the near-wall region. Therefore, the use of a multilevel approach comes as an alternative for modeling the corrosion phenomena in fluid dynamic systems.

5. ACKNOWLEDGEMENTS

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6. REFERENCES

Abe, K.; Kondoh, T., Nagano, Y., 1994. “A new turbulence model for predicting fluid flow and heat transfer in separating and reattaching flows. I. Flow field calculations”. *International Journal Heat Mass Transfer*, vol. 37, p. 139-151.

Balsara, D. S., 2001. “Divergence-Free adaptive mesh refinement for magnetohydrodynamics”. *Journal of Computational Physics*, vol. 174, p. 614-648.

Courant, R.; Friedrichs K.; Lewy, H., 1967. “On the partial difference equations of mathematical physics” . *IBM Journal of Research and Development*, v. 11, n. 2, p. 215–234.

Keating, A. 1999. *A model for the investigation of two-phase erosion-corrosion in complex geometries*. (Master of Engineering Science) – University of Queensland.

Kubrak, B.; Herlina, H.; Greve, F.; Wissink, J.G., 2013. “Low-diffusivity scalar transport using a WENO scheme and dual meshing”. *Journal of Computational Physics*, vol. 240, p. 158-173.

Lin, C. H.; Ferng, Y. M.,2014. “Predictions of hydrodynamic characteristics and corrosion rates using CFD in the piping systems of pressurized-water reactor power plant”. *Annuals of Nuclear Energy*, vol. 65, p. 214-222.

Nesic, S.; Postlethwaite, J.; Bergstrom, D. J.,1992. “Calculation of wall-mass transfer rates in separated aqueous flow using a low Reynolds number *k*-ε model”. Int. J. Heat Mass Transfer, vol. 35, no. 8, p. 1977-1985.

Ostilla-Monico, R.; Yang, Y.; Poel, E.P. V. D.; Lohse, D.; Verzicco, R., 2015. “A multiple-resolution strategy for Direct Numerical Simulation of scalar turbulence”. *Journal of Computaional Physics*, vol. 301, p. 308-321.

Panda, A.; Peters, E. A. J. F.; Baltussen, M. W.; Kuipers, J. A. M., 2019. “Fully resolved scalar transport for high Prandtl number flows using adaptive mesh refinement”. *Chemical Engineering Science*: X. vol. 4.

Poulson, B., 2014. “Predicting and preventing flow accelerated corrosion in nuclear power plant”. *International Journal of Nuclear Energy*, vol. 2014. 2014.

Prasad, M.; Gopika, V.; Sridharan, A.; Parida, S., 2018. “Pipe wall thickness prediction with CFD based mass transfer coefficient and degradation feedback for flow accelerated corrosion”. *Progress in Nuclear Energy*, vol. 107, p. 205-214.

Sydberger, T.; Lotz, U., 1982. “Relation between Mass-transfer and corrosion in a turbulent pipe-flow”. *Journal of the Electrochemical Society*, vol. 129. p. 276.

Xiong, J.; Koshizuka, S.; Sakai, M., 2011. “Turbulence modeling for mass transfer enhancement by separation and reattachment with two-equation eddy-viscosity models”. *Nuclear Engineering and Design*. vol. 241. p. 3190-3200. 2011.

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