

Comparative analysis of CFD models to simulate temperature non-uniformity during hydrogen tank refuelling

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ABSTRACT

This study compares four computational fluid dynamics (CFD) models, i.e. k- ϵ , RSM, SAS, and LES, to simulate temperature non-uniformity during hydrogen tank refuelling. Three grids with a total number of control volumes of 64k, 363k, and 2.9 M were used. The maximum dimensionless wall distances, y^+ , were 80, 5 and 2.5, respectively. The predictive capability of the models was assessed by recommended statistical indicators using ten thermocouple locations during 620 s of the experiment. The comparative analysis demonstrated a better predictive capability of temperature non-uniformity and stratification by the LES model and a shorter simulation time. It is concluded that meshes with y^+ larger than 80 would overpredict the average hydrogen temperature while meshes with $y^+ < 5$ provide a good simulation accuracy. The results underline the importance of the turbulence model choice and the numerical grid resolution for proper prediction of temperature non-uniformity during hydrogen tank refuelling.

1. Introduction

Composite tanks for high-pressure gaseous hydrogen storage combine acceptable energy storage density, matured manufacturing technology and affordable cost making them widely used in transport applications [1]. However, the temperature rise in the tank during refuelling brings safety concerns [2,3]. International regulation GTR#13 [4] requires that hydrogen bulk temperature in the tank should be between -40°C and $+85^\circ\text{C}$. Many previous investigations, including the reduced model [5,6], experiments [7] and computational fluid dynamics (CFD) models [8,9] were focused on the assessment of the bulk (averaged) hydrogen temperature in a tank. Unfortunately, the problem of temperature non-uniformity inside the tank has been left out of regulations, codes, and standards (RCS) and requires more pre-normative research.

Experimental studies proved that temperature non-uniformity during the refuelling process can be significant, which highlights the importance of developing contemporary refuelling models capable of predicting, along with other parameters, the temperature distribution inside the storage tank, including hydrogen, liner and composite. In 2007, Dicken and Mérida demonstrated for the first time in their refuelling experiments [10] a vertical thermal stratification (8°C across the tank diameter) inside a horizontal 74 L volume tank instrumented with

63 internal thermocouples. They found the temperature distribution became more and more stratified vertically after extending the fuelling time, i.e., using lower gas velocities at the inlet. In 2008, Tera et al. [11] experimentally studied the impact of the inlet diameter and velocity on hydrogen temperature non-uniformity in the tank of 65 L volume with length-to-diameter ratio $L/D = 2.1$. The authors found that the vertical temperature gradient appeared when the gas inlet velocity was below 5 m/s. In 2010, Demaël et al. [12] experimentally observed a temperature gradient in the horizontal direction between the front and back side of a horizontally located 46 L tank with a comparatively large $L/D = 6.2$. They measured a temperature difference of 55°C at the beginning of the filling for a 15 MPa/min pressure ramp rate, and of around 30°C for a smaller 2.1 MPa/min pressure ramp rate. In 2017, Bourgeois et al. [13] confirmed the 5 m/s velocity criterion for gas stratification with both experiments and CFD in four tanks with an $L/D = 2.0$ – 5.4 and volume of 37–531 L. The authors observed that gas stratification appeared when the inlet gas velocity decreased below 5 m/s during the refuelling process. They also suggested that the injection velocity shall be below 100 m/s to avoid a horizontal temperature gradient for tanks with $L/D > 3$. In 2018, Bourgeois et al. [14] reviewed and discussed three phenomena leading to temperature heterogeneity: the lowest temperature near the inlet, the vertical temperature gradient inside the gas (thermal stratification), and the horizontal temperature gradient in tanks with an $L/D >$

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3. In 2023, Gebhart et al. [15] refuelled two tanks with the same inner and outer diameter and the same pressure ramp, but with different volumes and L/D (tank with volume 15.7 L and L/D = 3.3, and tank 38.7 L and L/D = 6.9). The hydrogen gas temperature distribution inside the tanks was measured by 8 thermocouples (TCs). During refuelling, the tank with L/D = 3.3 has a hydrogen temperature non-uniformity of 0–7 °C, while the tank with larger L/D = 6.9 has essentially higher hydrogen temperature non-uniformity of 10–25 °C.

Experimental investigation of temperature non-uniformity in a hydrogen storage tank is limited by difficulties in deploying and positioning TCs inside the tank, the number of TCs and the uncertain effect of TC rake (or rakes) on temperature and velocity fields. Three-dimensional (3D) CFD modelling is a non-disruptive research methodology that naturally overcomes the above experimental shortcomings and offers insights into details of temperature and velocity fields in the tank, including hydrogen and tank components (liner, bosses, composite wall). However, for CFD models to be a reliable engineering tool, they must be validated against experimental data. The predictive capability of a CFD model depends on the applied sub-models, including turbulence models (which are expected to simulate the combination of laminar, transitional and turbulent flows), the equation of state, grid design, numerical methods, etc.

In 2013, Suryan et al. [16] compared the application for refuelling of four Reynolds Averaged Navier-Stokes (RANS) turbulence models, i.e. realizable k- ϵ , Renormalization Group (RNG) k- ϵ model, Reynolds Stress Model (RSM), and k- ω Shear Stress Transport (SST), using a two-dimensional (2D) axial symmetry CFD model. Though the authors concluded that the realizable k- ϵ and the RSM are the most suitable models, the simulation results with all four turbulent models were pretty much similar to each other with a temperature difference within 3 °C (~3% if compared to the maximum temperature of about 100 °C) and the advantage of RSM stated by the authors was not obvious. The 2D models have been later used by many other researchers [17–19] to investigate the temperature evolution inside the tank. Unfortunately, the use of 2D models to study 3D phenomena, e.g. refuelling with non-uniform temperature distribution, is questionable and thus the conclusions cannot be fully trusted. In 2014, Galassi et al. [20] claimed that the difference between temperature profiles simulated using the modified k- ϵ and SST models could be about 10% with 3D simulations, but no details were provided. In 2023, Xie et al. [21] compared the performance of five turbulence models, i.e. modified k- ϵ model, RSM, Scale-Adaptive Simulation (SAS), Detached Eddy Simulation (DES), and Large Eddy Simulation (LES), using 3D simulations. While all turbulence models correctly reproduced the experimentally measured averaged (the only parameter provided in the experimental paper [22]) hydrogen temperature history, essentially different dynamics of velocity and temperature fields inside the tank were observed between RANS (modified k- ϵ and RSM), hybrid (SAS and DES) and LES models.

A comparative analysis of four different real gas equations of state (EoS) for the simulation of refuelling of a Type III tank (up to 35 MPa) and a Type IV tank (up to 77.5 MPa) was performed by Suryan et al. [16] and Melideo et al. [22] in 2013 and 2014, respectively. The authors analysed modelling performance with Redlich-Kwong, Soave's modified Redlich-Kwong, Aungier's modified Redlich-Kwong and Peng-Robinson real gas EoS and did not find apparent differences. The use of the ideal gas law provided about 14° lower temperature than that obtained with the Aungier Redlich-Kwong real gas EoS [22]. In 2018, Bourgeois et al. [14] suggested that the National Institute of Standards and Technology (NIST) database would be the most accurate option to account for the real gas properties of hydrogen for refuelling simulations.

The best practices presume that CFD simulations should be accompanied by a grid independence study. However, its practical implementation in some cases may result in a prohibitively large number of control volumes (CVs) and unacceptably long CPU time [23]. Consequently, only a few authors reported consistent grid sensitivity analysis. For example, four grids having varying degrees of local refinement

around the pipe and gas/solid interface were used by Galassi et al. [20]. The authors demonstrated that the maximum hydrogen temperature deviation from experimental measurements was within 7% (compared to the maximum calculated temperature around 100 °C) for all grids. The effect of boundary layer resolution at the interface between hydrogen and tank wall was studied by Melideo et al. [24], and no impact on temperature distribution inside the tank was observed. It should be noted that both studies used the k- ϵ models.

Many of the early time CFD studies did not analyse temperature distribution inside the tank due to the absence of detailed experimental data. A recent experimental study [25] of hydrogen refuelling included tanks that were well-instrumented with TCs. The study reported spatial and temporal temperature distribution inside the tank. This allows to validate 3D CFD simulations against experimentally measured hydrogen temperatures in different tank locations. In 2023, Based on the refuelling experiments in a 36 L tank with an L/D = 2.4 [25,26], a comparative analysis of two turbulence models was published by Gonin et al. [27] using 3D simulations. As the inlet velocity was lower than 5 m/s, a significant vertical temperature gradient in the horizontally oriented tank was measured by ten TCs and was equal to 51 °C. This value was underestimated by 4% and 47% with the SAS (k- ω SST SAS) and the k- ω SST, respectively. The authors concluded that the use of the SAS turbulence model decreased the overprediction of simulated turbulence generation and underprediction of temperature non-uniformity. However, the CFD model was based on a number of assumptions and simplifications, e.g. the rod connecting TCs was neglected, and the SAS model was not used from the beginning of refuelling. Also, the grid sensitivity analysis was not reported. In 2024, Martin et al. [28] reported another refuelling experiment with a 165 L tank with L/D = 8.2, where dozens of TCs were used to measure the temperature of hydrogen and tank material. Compared to the experimental measures, the authors examined the performance of k- ϵ , k- ω SST, SAS and RSM turbulence models in 3D refuelling simulations. The experimentally measured temperature difference between two TCs in the liner (located at the top and bottom of the middle part of the tank respectively) at 3000 s (mass flow rate was 2 g/s for this comparatively large volume tank of 165 L) reached a significant value of 23 °C. This temperature difference was underestimated by 26%, 43% and 78% by the RSM, SAS, and k- ω SST models, respectively. The authors concluded that the RSM model was the best to represent the flow and thermal behaviour inside the tank during refuelling and that the k- ω SST model should be “disqualified” for refuelling simulations. However, the authors did not give an efficient quantitative comparison of the models' performance as a statistical analysis of solutions provided by different turbulence models and grids independence study was not performed.

The gas stratification will introduce a significant temperature nonuniformity inside the tank, which can increase the maximum hydrogen temperature above 85 °C in a standard fast fuelling process. So it is important to evaluate the ability of CFD models to predict gas stratifications during a fuelling process. Our previous work [21] has proved that all five turbulence models (RSM, DES, SAS, LES and k- ϵ) can well predict the hydrogen temperature without gas stratification. As a supplement work, this paper aims to investigate the effects of CFD model parameters, including turbulence models (RSM, SAS, LES and k- ϵ), grid resolution, and time step on predicting a significant temperature non-uniformity (caused by gas stratification) inside the hydrogen storage tank in the well-instrumented experiment by Gonin et al. [26]. To underpin the credibility of conclusions on the predictive performance of different models, the simulations will be statistically analysed using methods well-established in the CFD community.

2. Validation experiment

The well-instrumented refuelling experiment published in the HyTransfer project report [25] and Gonin et al. paper [26] are used for validation of simulations in this study. The vessel used in the experiment

Table 1

Geometry and material properties of the experimental Type IV tank [25,26] used for refuelling simulations.

Overall tank characteristics	
Volume (L)	36
External length (mm)	913
External diameter (mm)	325
Inlet diameter (mm)	10
Thickness of liner (mm)	3.8
Thickness of composite overwrap (mm)	27.8
Polymer liner properties	
Liner heat conductivity (W/m/K)	0.414
Liner specific heat capacity (J/kg/K)	1799
Liner density (kg/m ³)	914
Carbon fibre reinforced polymer (CFRP) overwrap properties	
Composite heat conductivity (W/m/K)	0.616
Composite specific heat capacity (J/kg/K)	783
Composite density (kg/m ³)	1365
Stainless Steel 316L Plug and pipe properties	
Metal heat conductivity (W/m/K)	16.2
Metal specific heat capacity (J/kg/K)	500
Metal density (kg/m ³)	7990
Aluminium 6601 Boss properties	
Metal heat conductivity (W/m/K)	167
Metal specific heat capacity (J/kg/K)	896
Metal density (kg/m ³)	2700

was a 36 L Type IV Hexagon Lincoln tank. The initial temperature of the tank, including hydrogen, and pressure inside the tank were 18 °C and 2 MPa respectively. The average hydrogen mass flow rate during the entire refuelling was 2 g/s. The refuelling period was about 630 s with the final pressure of about 71 MPa. To compare numerical simulations against the refuelling test, the experimentally recorded transients of the inlet temperature of precooled hydrogen after a heat exchanger, the pressure transient inside the tank, and the spatial distribution of hydrogen temperatures during the refuelling test [25,26] are digitised with an accuracy of 0.2 °C and 0.1 MPa respectively.

Details of the tank geometry and material properties are given in Table 1, where the tank geometry was digitised from the HyTransfer report [25] and the same material properties as Gonin et al. [26] are used. The uncertainty in tank length and diameter is within 1% while the uncertainty in the thickness of the carbon fibre reinforced polymer (CFRP) and liner is within 5–10%. Those two thicknesses are then further adjusted with a similar 36 L Type IV tank used in our previous studies [29–31].

Locations of ten TCs deployed inside the tank to measure the spatial

hydrogen temperature distribution in time are shown in Fig. 1, where the x- and y-coordinates are indicated at the hydrogen inlet on the left side.

Table 2 presents the x-, y- and z-coordinates of ten TCs in the experimental tank [25].

2.1. Computational domain and numerical mesh

The computational domain is composed of the metal boss and plug, TCs rod, polymer liner, CFRP and hydrogen. Altogether three numerical meshes were applied in simulations for a grid sensitivity analysis, i.e. Mesh#1, Mesh#2 and Mesh#2 with refinement (Mesh#2-level2). Fig. 2 shows the cross-section of the calculation domain for Mesh#1 and Mesh#2. Please note that some regions look black due to dense black mesh lines, such as the yellow liner part between CFRP and hydrogen. In all meshes, more CVs are used in the centre of the tank to resolve the released jet flow, which is key to heat transfer and mixing inside the tank. In this paper, the TCs rod is also resolved as it can disturb the released jet flow and increase the heat transfer to the atmosphere.

Table 3 shows the total number of CVs, characteristic CV size and maximum dimensionless wall distance $y^+ = \frac{y u_\tau}{\nu}$, where $u_\tau = \sqrt{\frac{\tau_w}{\rho}}$ is the friction velocity, τ_w is the wall shear stress, ρ is the fluid density, y is the absolute distance from the wall, and ν is the kinematic viscosity. The values of y^+ in the table are presented for the near-wall CVs in the refuelling pipe and in the tank.

Mesh#1 is a relatively coarse mesh with only 64,032 hexahedral CVs (35,184 in hydrogen, 8256 in CFRP, 8768 in liner, 5120 in boss and

Table 2

The coordinates of ten TCs inside the experimental tank [25].

Thermocouple Number	x-coordinate (mm)	y-coordinate (mm)	z-coordinate (mm)
TT760	330	115	0
TT761	390	–115	0
TT762	445	60	0
TT763	505	–60	0
TT764	565	115	0
TT765	625	–115	0
TT766	700	0	20
TT767	745	115	0
TT768	745	–115	0
TT769	780	0	20

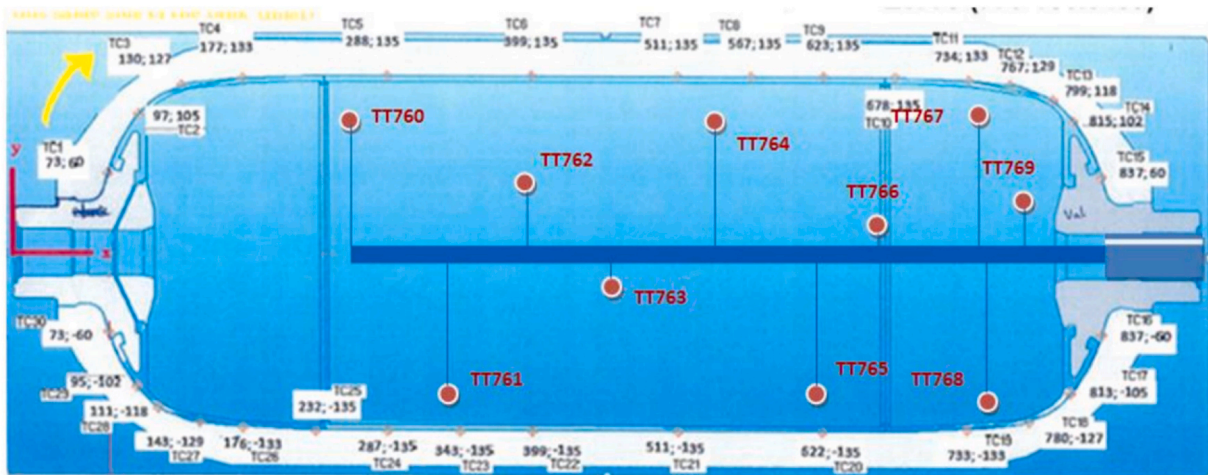


Fig. 1. Location of ten thermocouples in the experimental tank [25].

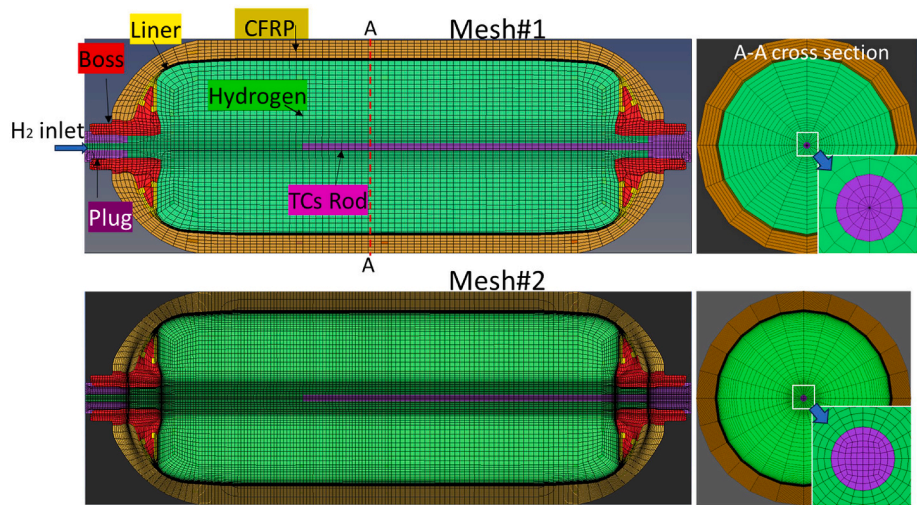


Fig. 2. Calculation domain and numerical Mesh#1 and Mesh#2 of 36 L Type IV tank.

Table 3
The number of CVs, minimum CV size and maximum dimensionless wall distance y^+ .

Mesh Name	Number of CVs	Minimum CV length	Maximum wall distance y^+	
			In pipe	In tank
Mesh#1	64,032	1.67 mm	120	80
Mesh#2	363,300	0.5 mm	50	5
Mesh#2-level2	2,906,400	0.25 mm	25	2.5

6704 in plug and TCs rod). There are 6 CVs across the inlet pipe of 10 mm diameter, giving the minimum CV size of 1.67 mm for this mesh. Mesh#2 has the increased CVs density in all directions with a finer mesh near the gas-solid interface (minimum CV size of about 0.5 mm with a growth rate of 1.25) with about 363,300 hexahedral CVs (179,232 in hydrogen, 71,208 in CFRP, 55,272 in liner, 27,024 in boss and 30,564 in plug and TCs rod). There are ten CVs across the inlet pipe diameter in Mesh#2. Mesh#2-level2 represents the global grid refinement of Mesh#2, which divides each cell by two in all three directions. For all meshes, the minimum orthogonal quality of CVs in fluid regions is 0.3–0.4, while 90% of CVs have a quality of 0.6–1.0. During the simulations with Mesh#1, the value of the maximum wall distance y^+ is around 120 in the pipe and 80 in the tank, while with Mesh#2, the maximum wall distance y^+ is around 50 in the pipe and 5 in the tank for all turbulence models. In this paper, we focus on the flow and mixing behaviour including the near-wall flow with no-slip conditions on the wall. Theoretically, the use of dimensionless distance $y^+ \sim 1$ is ideal for resolving the whole boundary layer. However, the use of smaller CV size to decrease y^+ would increase the simulation time to make it unreasonable. Here for meshes with $y^+ > 1$, a standard wall function is employed for the RSM, SAS and k- ϵ turbulence models and a near-wall treatment is used in LES simulations, where the laminar and logarithmic law-of-the-wall or their blending is employed with different y^+ [32]. The resolution of such a method has been tested by Salim and Cheah in their study on a wall-bounded flow in 2009 [33]. They demonstrated that meshes with $y^+ < 5$, when the laminar-law region is resolved, show the best result while meshes with $30 < y^+ < 60$, when the log-law region is resolved, are also sufficiently accurate compared to the experimental wall friction coefficient. Meanwhile, the authors proved and advised that meshes with $5 < y^+ < 30$, when the buffer region is

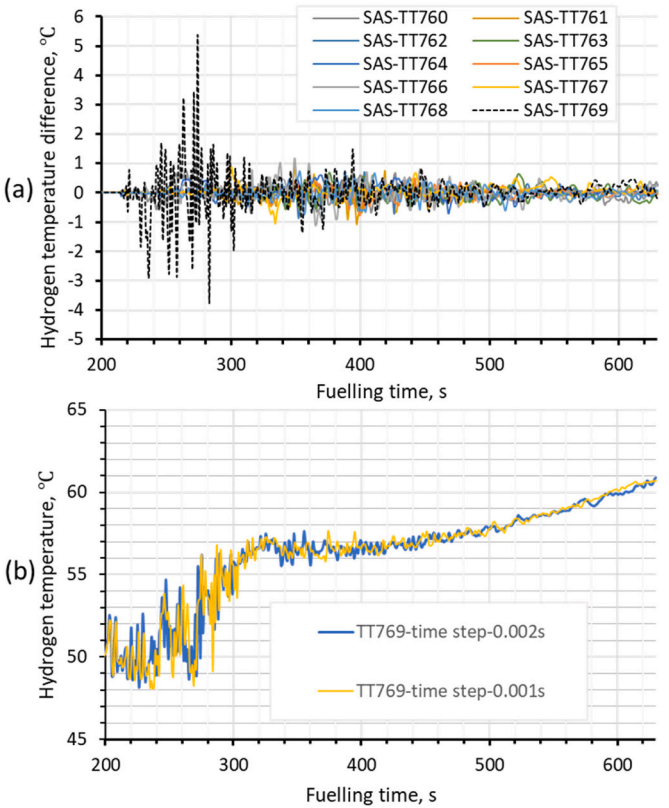


Fig. 3. Simulation results with the time step 0.002 s and 0.001 s (the SAS turbulence model, Mesh#2): (a) The difference of hydrogen temperature in locations of ten TCs; (b) The temperature dynamics simulated in the location of the “problematic” thermocouple TT769.

resolved, shall be avoided as neither wall functions nor near-wall modelling approach accounts for it accurately.

2.2. Governing equations, initial and boundary conditions

The governing equations of the CFD models employed in this study

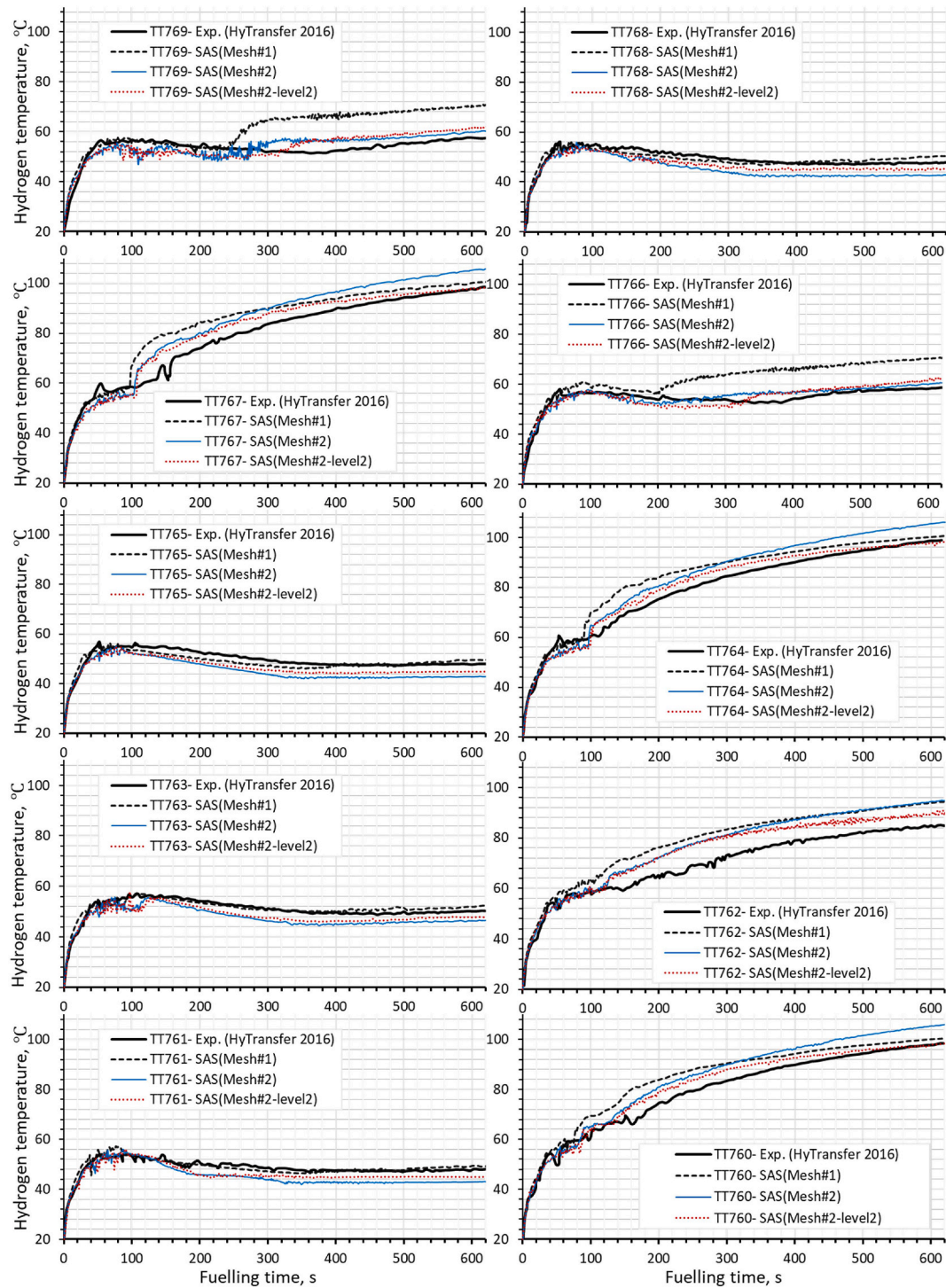


Fig. 4. The SAS model grid sensitivity: experimental temperature dynamics in the tank against simulated temperature with Mesh#1, Mesh#2, and Mesh#2-level2 (time step 0.002 s).

included 3D compressible mass, momentum, and energy conservation equations with details required for RSM, SAS, LES and $k-\epsilon$ turbulence models [34]. Descriptions of the models can be found elsewhere [21].

The initial and boundary conditions for simulations are the same as in the experiment by Gonin et al. [26]. The initial temperature of hydrogen and tank materials is equal to the ambient temperature of 18 °C, and the initial pressure in the tank is 2 MPa. A non-slip boundary condition is applied on all solid surfaces. The conjugate heat transfer

approach has been used to describe heat transfer between solid materials and hydrogen. The heat transfer coefficient on the outer surface of the tank to the atmosphere is assumed to be 6 W/K/m² [26,35].

The inlet hydrogen pressure P_{inlet} (MPa) and temperature T_{inlet} (°C) in simulations are approximated to experimental transients via polynomials with deviation from experiment ± 0.1 MPa and ± 1 °C respectively and used as the inlet boundary condition:

$$P_{\text{inlet}} = \begin{cases} 7.541799 \cdot 10^{-5} \cdot t^3 - 2.454048 \cdot 10^{-3} \cdot t^2 + 9.873172 \cdot 10^{-2} \cdot t + 2.034875, & (t \leq 26) \\ 1.109529 \cdot 10^{-1} \cdot t + 1.383734, & (t > 26) \end{cases} \quad (1)$$

$$\text{For } t \leq 9, T_{\text{inlet}} = 18, \quad (2)$$

$$\text{For } 9 < t \leq 367.86, T_{\text{inlet}} = 7.482119 \cdot 10^{-12} \cdot t^5 + 9.236679 \cdot 10^{-10} \cdot t^4 - 4.912091 \cdot 10^{-6} \cdot t^3 + 2.151379 \cdot 10^{-3} \cdot t^2 - 3.872621 \cdot 10^{-1} \cdot t + 20.89487, \quad (3)$$

$$\text{For } t > 367.86, T_{\text{inlet}} = 6.188786 \cdot 10^{-11} \cdot t^5 - 1.536808 \cdot 10^{-7} \cdot t^4 + 1.515832 \cdot 10^{-4} \cdot t^3 - 7.417808 \cdot 10^{-2} \cdot t^2 + 1.799985 \cdot 10^1 \cdot t - 1739.682, \quad (4)$$

where t is the refuelling time in seconds.

2.3. Numerical details

ANSYS Fluent 20.2 is used as a computational engine. The Pressure-Implicit with Splitting of Operators (PISO) scheme is applied as the pressure-velocity coupling method. A bounded second-order implicit scheme is chosen for time discretisation. The PRESTO scheme is chosen for the spatial discretisation of pressure while a second-order upwind scheme is chosen for the spatial discretisation of the rest parameters. As suggested by Bourgeois et al. [14], the National Institute of Standards (NIST) database is used to account for the real gas properties. The simulations started with a time step of 1×10^{-4} s and gradually increased by a factor of 1.005 after each time step until reaching the value of 2×10^{-3} s. This time step was chosen as the maximum to achieve the target equation residuals within 10–30 iterations per time step while minimising the overall CPU time. The convergence of linear equations solution was controlled requiring all residuals to be below the 10^{-3} threshold. The continuity equation residual reached this 10^{-3} threshold last and by that time the momentum conservation equation residual was reaching a value around 10^{-6} . The hydrogen mass balance, which was calculated by comparing the sum of the initial hydrogen mass in the tank plus hydrogen supplied to the tank to the current hydrogen mass in the tank, was within 0.1%.

3. Results and discussion

The sensitivity of simulations to the time step size (Courant–Friedrichs–Lewy, CFL, stability condition on a selected grid) is checked first to ensure that sufficient accuracy to reproduce experimental data is reached. Then, using the fixed time step size, the grid sensitivity for all three models is analysed (the k- ϵ model was not studied on Mesh#2-level2). The performance of different models to reproduce experimental data is discussed afterwards. Finally, statistical indicators are used as a statistical measure for quantitative comparison of the combined effects of grids, time steps, and turbulence models on the overall performance of the models to predict experimental data.

3.1. CFL number sensitivity

Here we use the convective cell $CFL = \frac{dt \cdot \sum_f \text{facial flux}}{2 \cdot V_{\text{cell}}}$, where dt is the time step, V_{cell} is the volume of CV, $\sum_f \text{facial flux}$ is the sum of absolute volume flux through all faces. The selected time step of 0.002 s corresponds to a maximum value of the CFL number of 6–60 in the pipe and 3–6 in the central region of the jet for Mesh#1 and Mesh#2 at the start of the refuelling simulations. The CFL number decreases with increasing refuelling time and ca. 95% of CVs inside the tank have a CFL below 1.

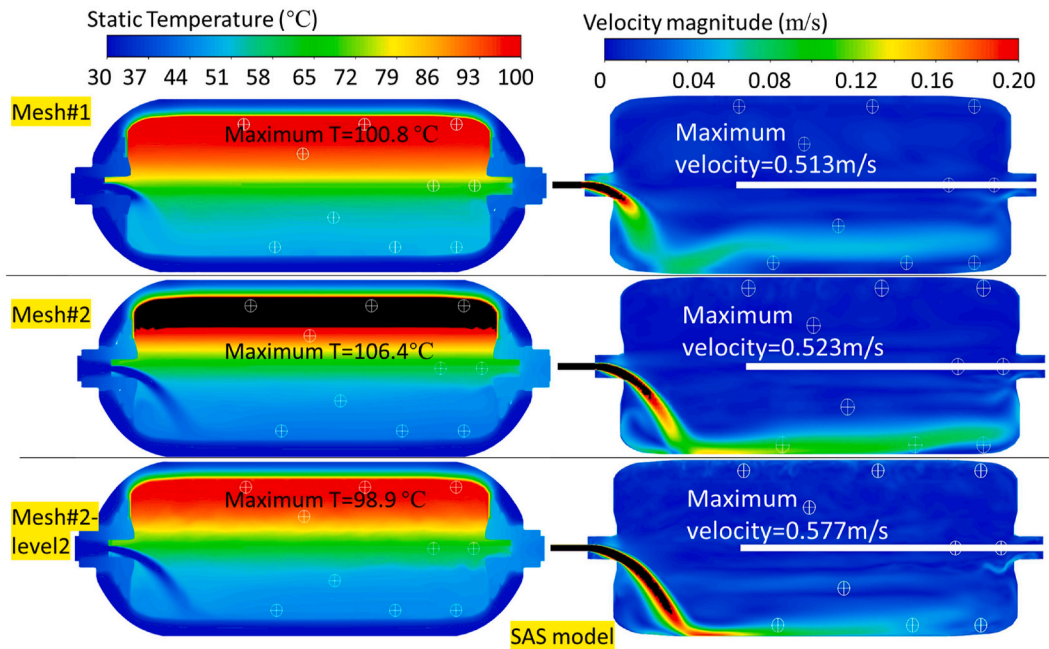


Fig. 5. The SAS model grid sensitivity: temperature and velocity distribution in the tank at the end of refuelling (620 s) with Mesh#1, Mesh#2, Mesh#2-level2 and time step 0.002 s.

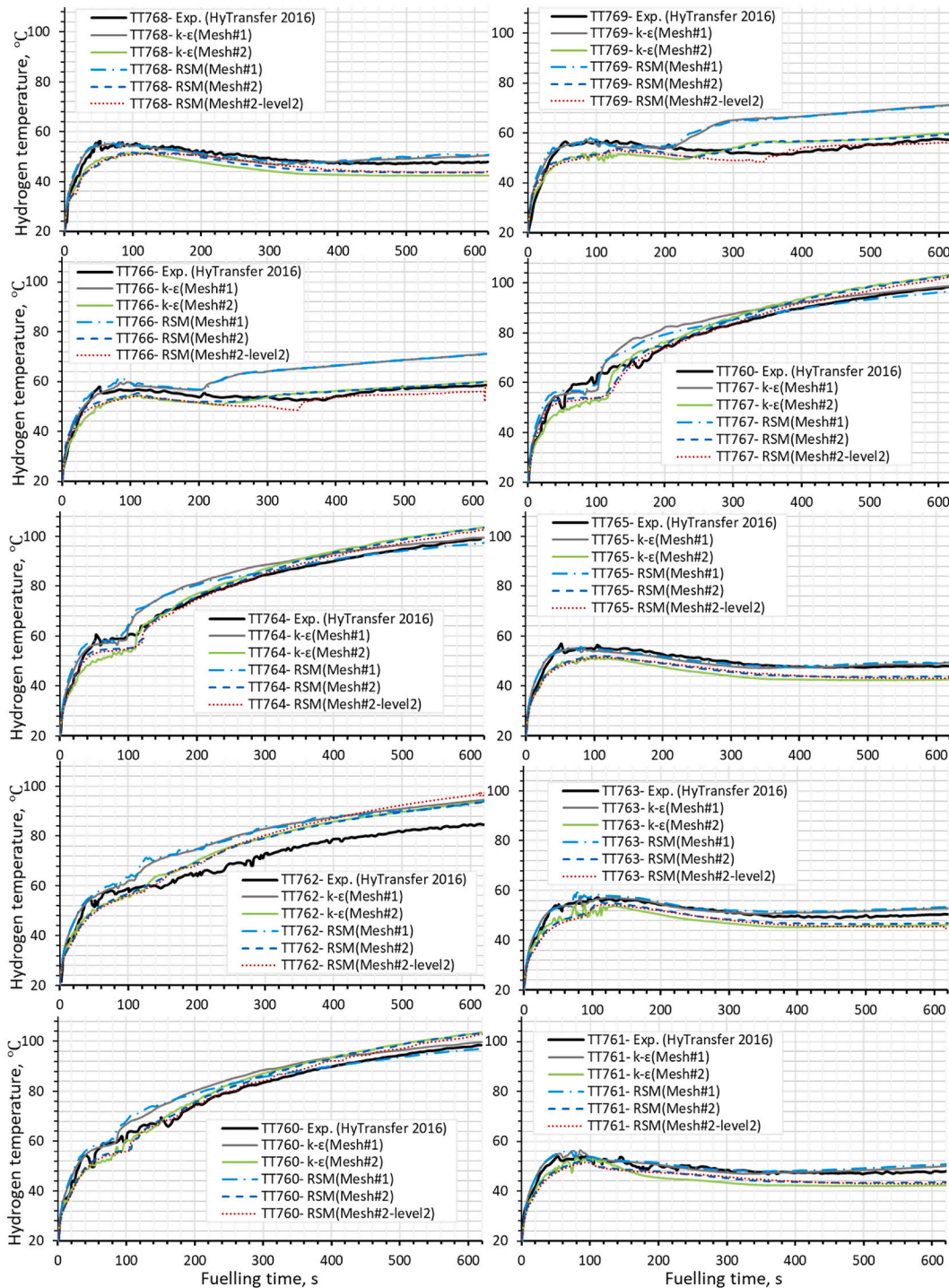


Fig. 6. The grid sensitivity of $k-\epsilon$ and RSM models: experimental temperature dynamics in the tank against simulated temperature with Mesh#1, Mesh#2, and Mesh#2-level2 (time step 0.002 s).

To test the CFL sensitivity of simulations to the prediction of temperature non-uniformity, the SAS model was rerun on Mesh#2 with a smaller time step of 0.001 s. This reduces the original cell convective CFL number, which corresponds to a maximum CFL of 60 in the pipe and 6 inside the tank, by half. To save the computational time, the test simulations start after a refuelling time of 215 s when the temperature non-uniformity becomes significant.

Fig. 3(a) shows the difference between simulated temperatures obtained with time steps 0.002 s and 0.001 s for all locations of ten TCs. The maximum difference in the temperature transients is within 1° (or

about 3% of the measured temperature rise in the tank of 37°C , from the initial 18°C – 55°C) except for TT769 (located at the end of the tank opposite to the hydrogen supply side), where short duration deviations up to $+5.5^\circ\text{C}$ and down to -4°C (about 15% of the experimental temperature rise of 37°C) are observed in simulations during period 200–300 s. However, the temperature difference between the two solutions oscillates around zero, i.e. indicating “no difference in average”. Those differences can be neglected if averaged through the whole refuelling time.

Fig. 3(b) shows the comparison of temperature dynamics simulated

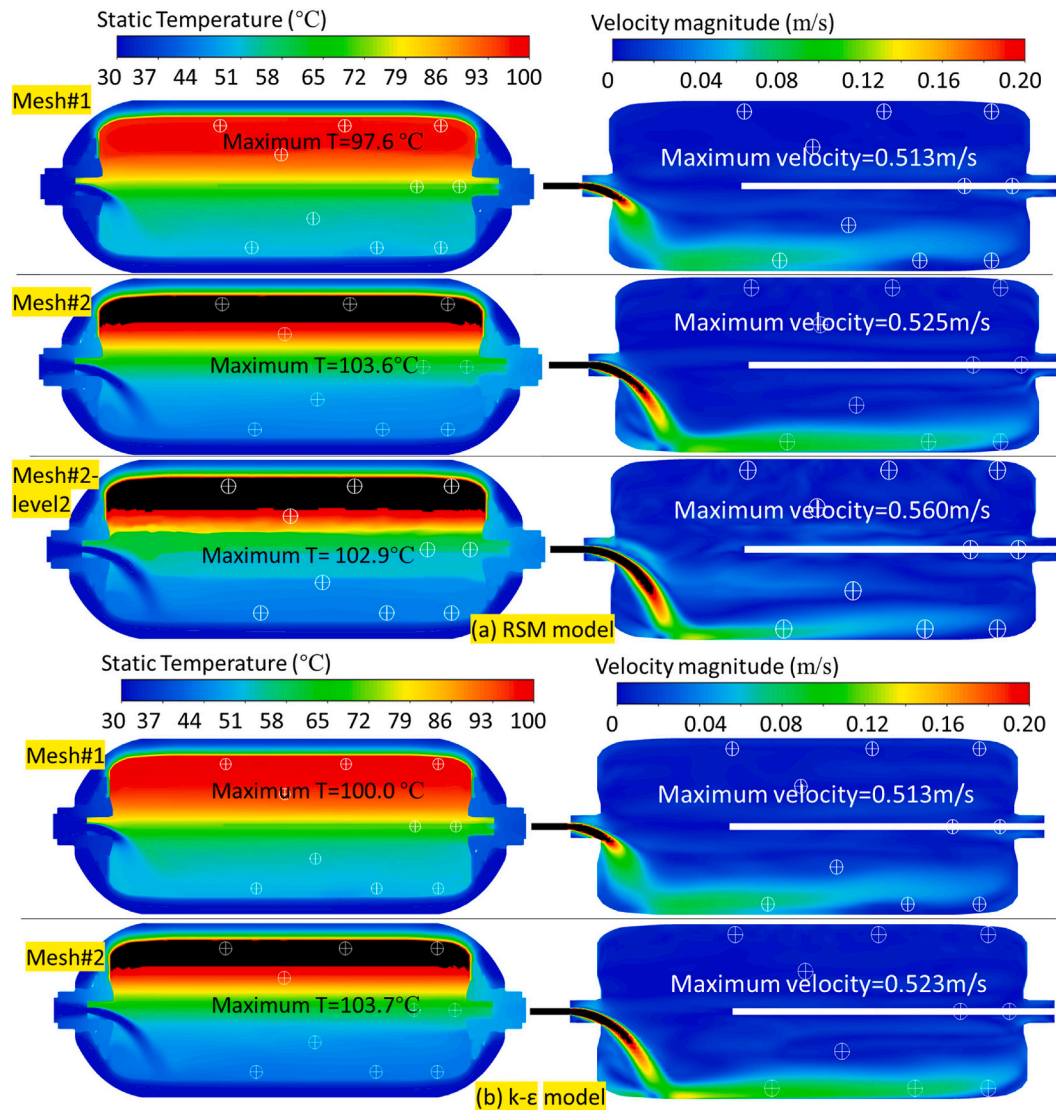


Fig. 7. Grid sensitivity for (a) the RSM model with Mesh#1, Mesh#2, and refined Mesh#2-level2 and (b) the k-ε model with Mesh#1 and Mesh#2 (time step 0.002 s): temperature and velocity distribution in the tank at the end of refuelling (620 s).

in the location of the “problematic” thermocouple TT769 using both time steps. The maximum and minimum temperatures in oscillation peaks are much closer to each other than 5.5 °C, which is caused by a misalignment of temperature dynamics in time. Moreover, the changes in the averaged statistical indicators over ten TCs are within 1% after reducing the time step, which proves the solution convergence at CFL number below 30–60 in the pipe and 3–6 inside the tank. The same CFL condition can be satisfied for all three meshes with the time step size of 0.002 s. So, the maximum time step is fixed at 0.002 s for the rest simulations in the study. Please note that using a larger time step of 0.004s will increase the continuity equation residual above 10^{-3} , which damages the mass conservation. Moreover, it will not speed up the simulation much as more iterations will be needed in each time step.

3.2. Grid sensitivity and model performance

To test the grid sensitivity, three meshes presented in Tables 3 and i. e. Mesh#1, Mesh#2 and Mesh#2-level2, are used with a fixed maximum time step size of 0.002 s for all simulations presented below.

3.3. SAS model

The influence of the numerical grid resolution on temperature dynamics with the SAS turbulence model is shown in Fig. 4.

Fig. 4 shows the comparison of simulated temperature dynamics with experimental temperature transients on three different meshes. Even the coarsest Mesh#1 with the maximum $y^+ \approx 80$ provides a reasonable temperature distribution inside the tank with time. The main disadvantage of the SAS simulations with Mesh#1 is the overprediction of temperatures in the middle of the tank by the height at the tank part opposite to the hydrogen supply pipe, i.e., in TT766 and TT769. The difference can be up to 14 °C (24%) at the end of refuelling. Mesh#2 with $y^+ < 5$ reduces this difference from 24% to 7%. However, Mesh#2 tends to overpredict the temperature gradient caused by gas stratification inside the tank. The temperatures at the top of the tank (TT760, TT762, TT764 and TT767) are still overestimated by 6–10 °C (7%–12%), while temperatures at the bottom (TT761, TT763, TT765 and TT768) are underestimated by 3–5 °C (7%–10%). With a globally refined Mesh#2-level2, which divides each cell by two in all three directions, there is only a slight improvement (about 1 °C, or 2%) in the predicted temperature history before the time of 300 s. The improvement becomes more pronounced by the end of refuelling (about 8 °C or 8% on TT760),

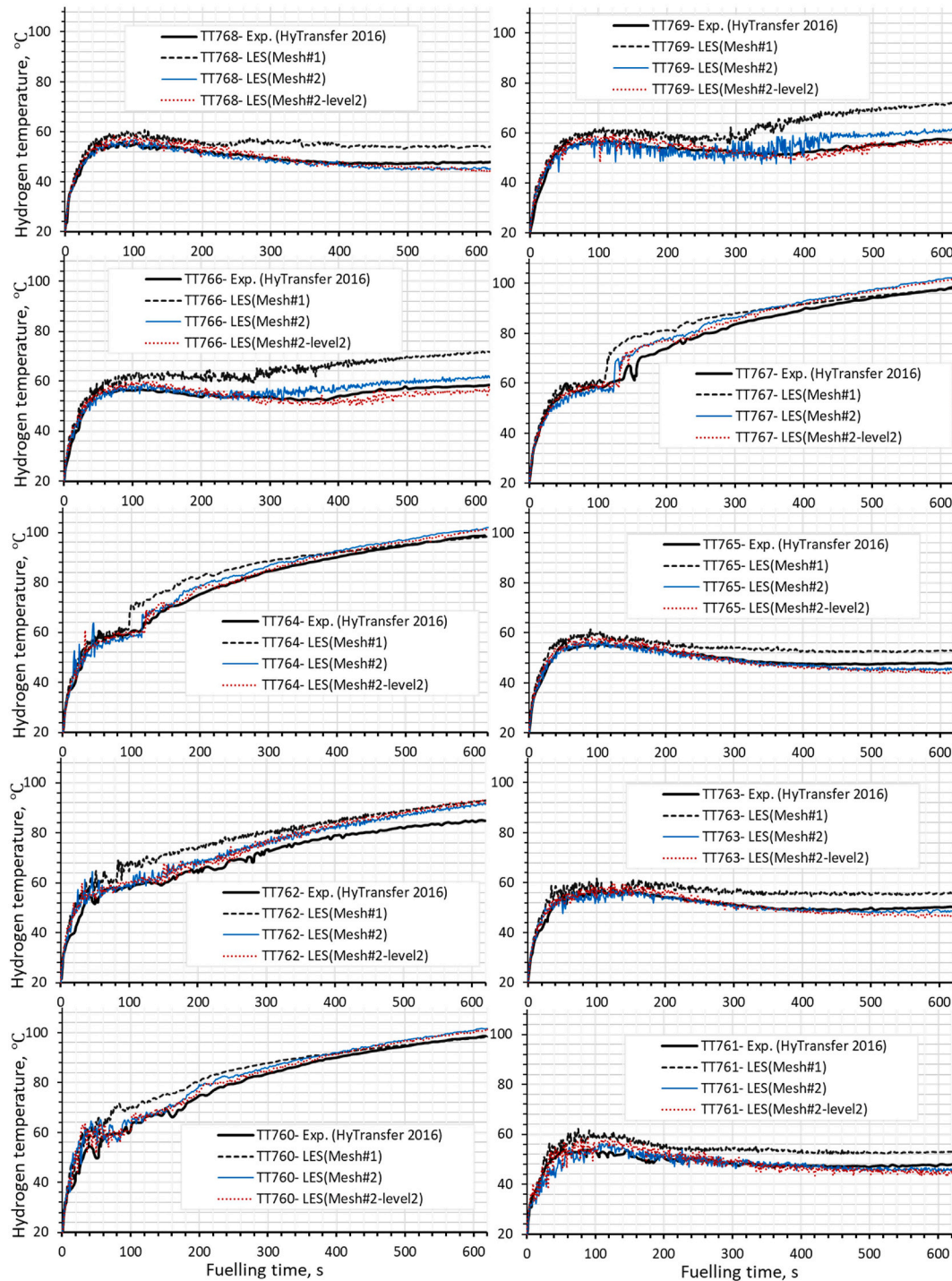


Fig. 8. The LES model grid sensitivity: experimental temperature dynamics in the tank against simulated temperature with Mesh#1, Mesh#2, and Mesh#2-level2 (time step 0.002 s).

where the vertical temperature gradient is reduced and becomes closer to the experiment.

Fig. 5 presents temperature and velocity fields by the end of refuelling at 620 s in the tank's central cross-section by the SAS model.

The temperature and velocity scales in Fig. 5 are limited by 30–100 °C and 0.00–0.20 m/s respectively and black colour in the field distributions indicates areas with temperature and velocity outside of these limits. The velocity of hydrogen supply decreases with an increasing fuelling time and falls in the range of 0.5–5 m/s after a

fuelling time of 80 s, i.e., below threshold 5 m/s that is “responsible” for vertical temperature stratification.

All three grids can capture the same flow pattern. As Mesh#1 is the coarsest grid near the wall (maximum $y^+ \approx 80$), it results in the horizontal jet detaching from the wall at the bottom and getting closer to the centreline of the tank compared to results on two other finer grids. It may overestimate the gas mixing in the tank due to “better entrainment” and overpredict the temperature in the centre of the tank. Mesh#2 has a finer grid near the wall (maximum $y^+ \approx 5$), which resolves the jet flow

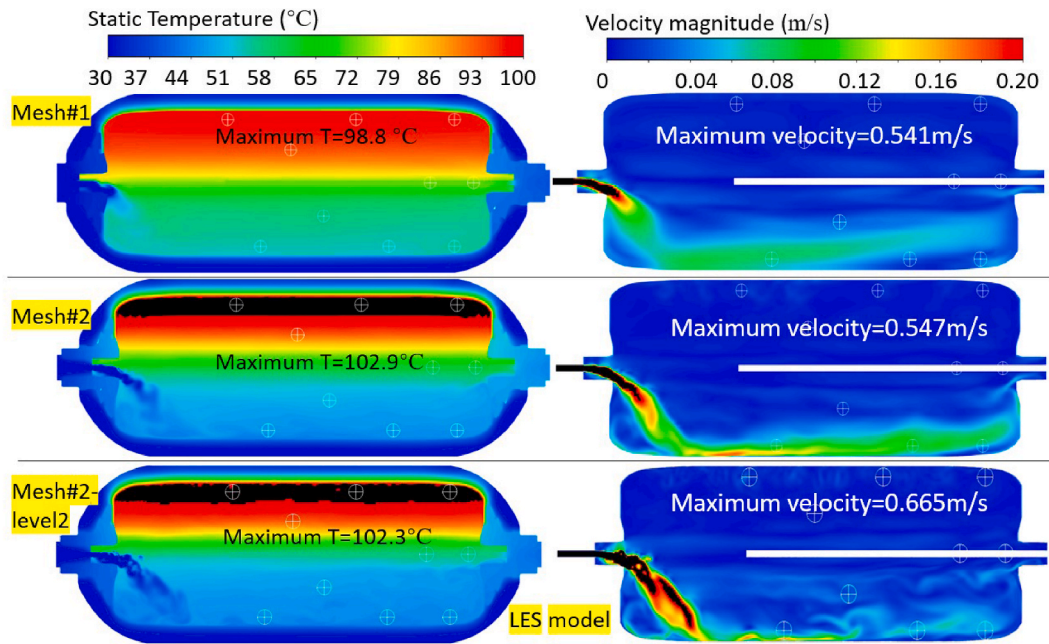


Fig. 9. The LES model grid sensitivity: temperature and velocity distribution in the tank at the end of refuelling (620 s) with Mesh#1, Mesh#2, refined Mesh#2-level2 and time step 0.002 s.

near the wall and avoids the jet detachment. However, the vertical hydrogen temperature gradient is more significant than on Mesh#1. Mesh#2-level2 (maximum $y^+ \approx 2.5$) has a doubled grid resolution in all directions, which gives a better resolution of the temperature and velocity fields and a closer prediction of experimental temperature distribution in time and space. We can see the convective flow near the top wall is better resolved on Mesh#2-level2 than on Mesh#2, which may account for the improvement of the predicted maximum hydrogen temperature.

3.4. RSM and $k-\epsilon$ models

The influence of the grid on the RSM and $k-\epsilon$ model simulations is shown in Fig. 6.

Like the SAS model, the RSM model with Mesh#1 overpredicts temperatures in “remote” locations TT766 and TT769 by up to 24% at the end of refuelling while with Mesh#2 it gives a better prediction (overprediction by no more than 10%). Except for the location TT762, the RSM simulations with Mesh#2 can predict the final temperature with a deviation within ± 5 °C. There is almost no difference between the RSM simulations with Mesh#2 and Mesh#2-level2, which indicates the achieved grid independence for this particular model. Unfortunately, the RSM model with both Mesh#2 and Mesh#2-level2 tends to underestimate the temperature in all locations by up to 16% in the period of 50–100 s.

The $k-\epsilon$ model performance is close to the RSM model with both Mesh#1 and Mesh#2 (no simulations were performed for the $k-\epsilon$ model for Mesh#2-level2). Their temperature histories almost coincide with each other in most TCs, see for example TT766 and TT769. Temperature and velocity fields at the end of refuelling are also nearly identical between the RSM and the $k-\epsilon$ models for Mesh#1 and Mesh#2 (see Fig. 7 (a) and (b) for RSM and $k-\epsilon$ model results respectively).

3.5. LES model

The influence of grid resolution on spatial and temporal temperature transients with the LES model is shown in Fig. 8.

While the LES model with Mesh#1 overestimates temperature in all locations by up to 27% at the end of refuelling, simulations with Mesh#2

reach an excellent agreement with the experiment with deviation of temperature from experiment no more than 8% at the end of refuelling. No significant improvement of the simulation results is observed after further global mesh refinement, and the LES model with Mesh#2-level2 ($y^+ \approx 2.5$) only slightly improves the results on Mesh#2 ($y^+ \approx 5$) in TT769 and TT766. Those two TCs are located near the end of the jet flow, where vortexes occur (see the velocity contour in Fig. 9). Thus, they are more sensitive to the momentum loss and mixing behaviour of the jet from the upstream parts of the flow. Fig. 9 gives the velocity and temperature distributions for the three grids.

Fig. 9 demonstrates that Mesh#1 provides a smaller temperature gradient in the vertical direction in comparison with results obtained using Mesh#2 and Mesh#2-level2. The same is supported by temperature dynamics in Fig. 8, though by the end of refuelling the temperatures in upper locations TT760, TT764 and TT767 are nearly equal to the experimental readings (less than 1 °C), the temperatures at the lower locations TT761, TT765 and TT768 are larger than in the experiment by about 5–7 °C (10–13%). Compared with Mesh#2, though a better velocity field resolution is achieved with Mesh#2-level2 as expected, the temperature difference is negligible.

3.6. Comparison of the bulk hydrogen temperatures and average heat flux

For all simulations, they have the same pressure histories inside the tank as a pressure inlet boundary condition is used. For the inlet mass flow rate of hydrogen, there is a small difference of 1–3% between simulations with different meshes. This is mainly caused by the tiny variation of the tank volume and inlet area in numerical simulations with different grid resolutions. Such a small variation in the tank volume has a very limited influence on the mass-averaged hydrogen temperature, which is mainly affected by the pressure ramp.

Fig. 10 shows the mathematical average hydrogen temperature measured at the same locations of ten TCs for all simulated cases. All simulations with Mesh#1 overestimate the average hydrogen temperature by 4–6 °C (6–10%). It is thought due to a large dimensionless wall distance with $y^+ \approx 80$. The coarse mesh reduces the heat transfer from compressed hotter hydrogen to the tank wall. The LES model shows 1–2 °C degrees higher deviations compared to other models on the coarse Mesh#1. On Mesh#2 with $y^+ < 5$ in the tank, all models get a

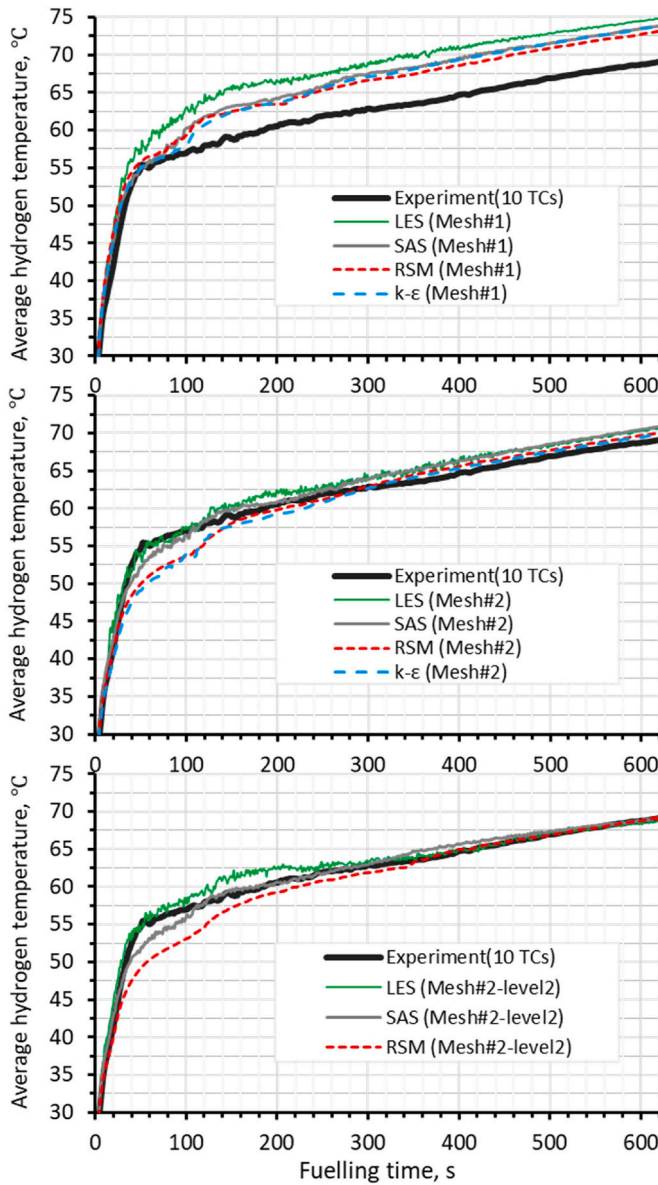


Fig. 10. Mathematical average hydrogen temperature over ten TCs for all cases and the experiment: top – Mesh#1, middle – Mesh#2, bottom – Mesh#2-level2.

temperature closer to the experiment by the end of refuelling with a 1–2 °C higher than in the experiment. The LES model gives the best performance in the first 100 s and somewhat overestimates the final temperature by around 1%, which is within the experimental error. The SAS model performs close to LES on the prediction of average temperature. The RSM and k-ε models show similar results to each other, both give quite accurate final temperatures but underestimate the hydrogen temperature by 4–6 °C (8–12%) in the first 100 s. The use of the finest Mesh#2-level2 brings a change within 1–2% in the average hydrogen temperature for LES, SAS and RSM, and the experimental temperature at the end of the process is reproduced with high accuracy.

The increase of average temperature in simulations compared to the experiment can be explained by the difference in the simulated area-weighted average heat flux (here, the area of the CV surface where the heat flux happens is considered) from hydrogen to the tank liner shown in Fig. 11. For all models, the average heat flux has the lowest value for the coarse Mesh#1. For example, the LES model gives 6–9% smaller total heat flux on Mesh#1 compared to Mesh#2 and Mesh#2-level2 during the whole refuelling time. We also note that the heat flux is

overestimated by the RSM and k-ε models on Mesh#2, which decreases their average hydrogen temperature at the beginning of fuelling.

3.7. Statistical comparison of different models to predict experimental data

It is not possible to objectively assess “by eyes” the predictive capability of the model by looking at temperature profiles in different TCs locations during the entire refuelling process. The international CFD community developed Statistical Performance Measures (SPMs) to provide rigorous means of quantitative CFD model evaluation and comparison of predicted and measured physical parameters [36]. A few commonly used dimensionless statistical indicators are used here to evaluate the model’s accuracy.

The Mean Relative Bias (MRB) suggested by the European project SUSANA [36] indicates a model’s ability to predict the measured values on average, and its sign shows whether the model is under- or over-predicting experimental data:

$$MRB = \frac{1}{N} \sum_{t=1}^N 2 \frac{T_{CFD,t} - T_{Exp,t}}{T_{CFD,t} + T_{Exp,t}}, \quad (5)$$

where $T_{CFD,t}$ and $T_{Exp,t}$ represent simulated and experimental temperatures at time t respectively (in °C), and N is the number of data points. However, under- and over-predictions cancel each other out and a model may appear to perform well for the wrong reason. Therefore, MRB is suggested to be paired with other model performance indicators, such as the Mean Relative Square Error (MRSE) [36], which sums the squares of the errors and therefore gives an indication of the scatter in the predictions:

$$MRSE = \frac{1}{N} \sum_{t=1}^N \left(2 \frac{T_{CFD,t} - T_{Exp,t}}{T_{CFD,t} + T_{Exp,t}} \right)^2. \quad (6)$$

To calculate the indicators, $T_{CFD,t}$, temperatures in all ten TCs locations are recorded every second in the simulations, i.e., 6200 data points of temperature over the entire refuelling period of 620 s. For experimental temperatures, the value is first digitised from references [25,26], i.e., $[t_{dig}, T_{Exp,t,dig}]$ which is recorded at a different time t_{dig} . For data process, the data set of $[t_{dig}, T_{Exp,t,dig}]$ is then linearly interpolated into $[t, T_{Exp,t}]$. The average deviation caused by the interpolation is below 0.1 °C and can be neglected compared to the difference between simulated $T_{CFD,t}$ and experimental $T_{Exp,t}$ temperatures.

Table 4 shows details (turbulence model and mesh) and results (CPU time and indicators) for all 11 simulated refuelling cases sorted by the values of MRSE from small to large.

The values of MRB confirm that all models with the coarsest Mesh#1 ($MRB > 5\%$) tend to overestimate the average hydrogen temperature, among which LES shows the largest $MRB = 9.3\%$ on the coarsest grid. The global deviation decreases with refined Mesh#2 and Mesh#2-level2. The negative MRB values for the SAS, RSM and k-ε on Mesh#2 and Mesh#2-level2 ($-0.3\% < MRB < -3.0\%$) mean that the average temperature is slightly underestimated. All 11 simulated cases show a “good” performance, satisfying the quantitative criterion of $-0.4 < MRB < 0.4$ and $MRSE < 1.5$ [36]. Fig. 12 shows the plot of MRSE against MRB, where models with smaller values of MRSE represent better model performance.

Here we can see LES on Mesh#2 and LES Mesh#2-level2 give very close results to the perfect model while simulations on Mesh#1 give the farthest results. The good performance of LES with Mesh#2 proves its advantage in simulations where the flow is sufficiently resolved ($y^+ < 5$), and near-wall CV is in a laminar boundary layer region. It is worth mentioning that the LES model has a shorter simulation time than the k-ε and RSM models on the same grids with an equal number of computational cores. For the RANS model, k-ε gives a similar performance as RSM on Mesh#1, while RSM performs better on Mesh#2. It shall be

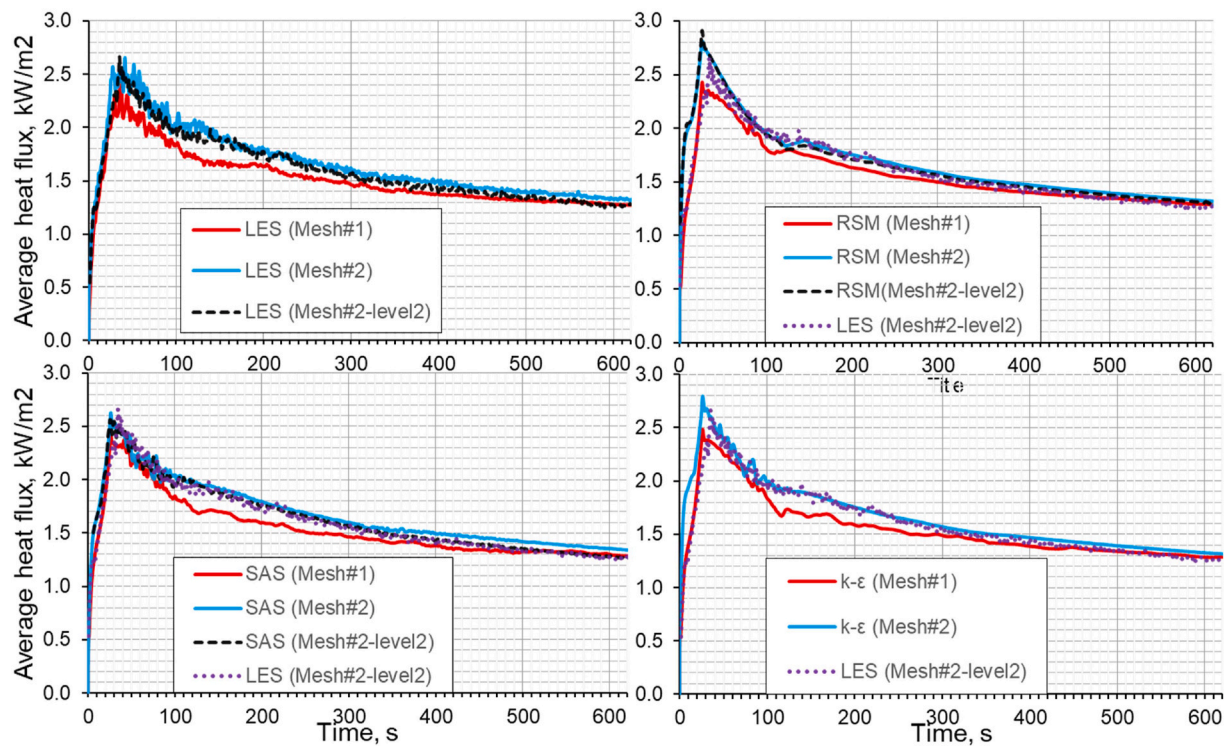


Fig. 11. Average heat flux from hydrogen to tank liner as a function of time for different turbulence models and meshes.

Table 4
Number of CPU cores, time and indicators for 11 simulated refuelling cases.

Turbulence model	Mesh	CPU cores	CPU time, days	MRB	MRSE
LES	Mesh#2-level2	256	30.4	0.9%	0.0010
LES	Mesh#2	128	10.4	1.5%	0.0011
SAS	Mesh#2-level2	256	32.1	−0.6%	0.0018
RSM	Mesh#2	128	13.5	−1.7%	0.0020
RSM	Mesh#2-level2	256	34.4	−3.0%	0.0023
k-ε	Mesh#2	128	11.1	−2.8%	0.0032
SAS	Mesh#2	128	9.9	−0.3%	0.0033
RSM	Mesh#1	64	4.1	5.7%	0.0042
k-ε	Mesh#1	64	4.1	5.5%	0.0042
SAS	Mesh#1	64	4.2	5.8%	0.0046
LES	Mesh#1	64	4.0	9.3%	0.0062

noticed that the SAS model did not provide an overall better solution than k-ε or RSM on Mesh#1 or Mesh#2. However, the SAS model gives slightly better results than RSM on Mesh#2-level2. This is probably because the scale equation of SAS models is based on an exact transport equation for the turbulence length scale [32], which is different from the simple dimensional arguments in classic RANS models and requires a higher grid resolution. (The same conclusions can be further confirmed with three other different statistical indicators in the supplemented material, which may offer more statistical information to readers.)

Finally, it could be concluded that the LES model, which is able to simulate the complex flows with a mixed laminar, transitional, and turbulent areas, is the best to accurately reproduce the experimental data at a shorter CPU time compared to other investigated models. All four turbulence models show poor performance on Mesh#1, which is caused by both lower grid resolution inside the tank and the under-prediction of heat flux from hydrogen to the tank. Thus Mesh#1 with a maximum dimensionless wall distance $y^+ \approx 80$ shall be avoided.

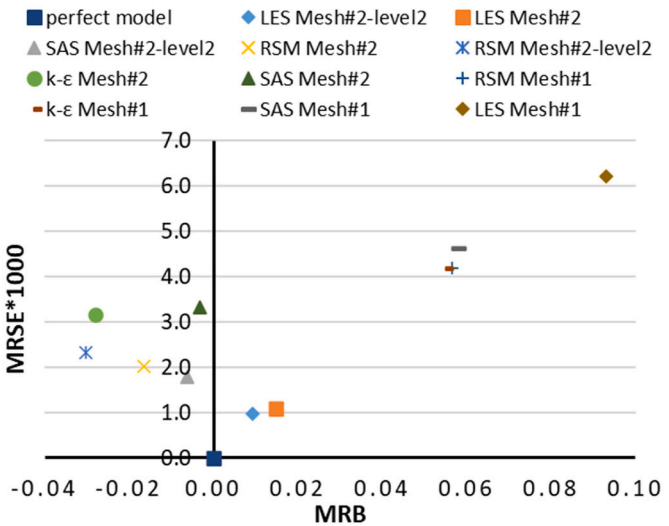


Fig. 12. Plots of MRSE against MRB

4. Conclusions

The *originality* of this study is in the comparative analysis of CFD model performance in 3D refuelling simulations to predict temperature nonuniformity. Four turbulence models (k-ε, RSM, SAS, LES) and three grids (Mesh#1, maximum $y^+ \approx 80$; Mesh#2, maximum $y^+ \approx 5$; Mesh#2-level2, maximum $y^+ \approx 2.5$) are investigated. The hydrogen temperature history, velocity and temperature fields are analysed. Statistical performance measures are used to quantitatively calculate the model accuracy for the refuelling simulations by comparing experimental measures on 10 TCs inside the tank. The comparative analysis confirms the advantage of the LES in predicting the temperature nonuniformity for refuelling processes with a significant gas

stratification while the performance of k- ϵ , RSM and SAS is found similar to each other on the same grid level. The result also shows that Mesh#1 with $y^+ \approx 80$ significantly overpredict the average hydrogen temperature inside the tank while Mesh#2 with $y^+ < 5$ and Mesh#2-level2 with $y^+ < 2.5$ reproduced it with good and high accuracy, respectively.

The *significance* of this work is in practical information on the accuracy of predictions of temperature distribution, which is directly relevant to the composite hydrogen storage tank safety. A detailed discussion on the flow and temperature field is provided, which visually shows the influence of grids and turbulence models. The obtained results provide insight for numerical modelling in tank design for mobile applications, development of refuelling protocols and carrying out safety engineering design of high-pressure hydrogen storage systems.

The *rigour* of this work is in the validation of refuelling simulations against experimentally measured temperature dynamics obtained from ten TCs positioned at various locations throughout the tank and the use of quantitative statistical analysis for comparison of the combined effect of turbulence models and numerical grids. Recommended statistical indicators are employed for the cumulative presentation of temperature prediction accuracy in all ten TCs and over the entire duration of the refuelling process of 620 s (6200 data points for each case) as a single value, which assures the proper assessment of the accuracy of the models.

5. Discussions

Numerous turbulence models have been used for refuelling simulations in different references. Readers may be confused by the choice of the right turbulence model. Combined with our previous study [21] on a standard fuelling process, where the gas stratification was not pronounced, the choice of turbulence model depends on the refuelling conditions.

For a refuelling process accompanied by a significant gas stratification, which can be caused by a slow inlet velocity, a large ratio of tank length/diameter, and so on. Due to the gas stratification, the flow inside the tank can be locally laminar or transitional. At the same time, the spatial temperature distribution becomes significant, which requires an accurate flow field to be solved. In such a situation, while RANS turbulence models tend to overestimate the turbulent mixing and heat transfer, LES gives a more accurate prediction.

For a standard fast refuelling without significant gas stratification, the temperature of hydrogen inside the tank is usually uniform due to a good mixing caused by a large jet velocity. Our previous work [21] using 3D simulations proved that all five turbulence models (RSM, DES, SAS, LES and k- ϵ) have quite similar performance. This is because the flow is fully turbulent and the spatial variation of hydrogen temperature caused by model choice can be neglected due to a global uniform hydrogen temperature distribution. However, it was found that the LES model and hybrid models are more sensitive to the time step and grid resolutions. Especially LES model requires a small CFL of approximately 1, which significantly increases the computational cost. Hence, classic k- ϵ and k- ω models may be a better choice in this case.

CRediT authorship contribution statement

Hanguang Xie: Investigation, Methodology, Writing – original draft. **Dmitriy Makarov:** Writing – review & editing. **Sergii Kashkarov:** Project administration, Writing – review & editing. **Vladimir Molkov:** Conceptualization, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2024.05.047>.

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