

On the reduced order modelling of Lithium-ion cells: comparison with higher order methods

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Abstract. Battery electric vehicles are the focus of major research and development efforts at several levels. In these vehicles, the energy storage system is still the limiting factor preventing widespread adoption. The thermal management of battery cells is a critical aspect of electric vehicle design as it affects the performance, the lifespan, and safe operation of battery packs. This work presents the development of thermal models of Lithium-ion cells arranged in a square lattice configuration. Initially, the battery pack arrangement is studied by developing a dedicated 2D CFD model encompassing half of the physical domain. Furthermore, results obtained by means of the adopted modelling strategy are compared with the outcomes of a reduced order model based on empirical correlations commonly used in these applications. Finally, strengths and weaknesses of the different approaches are highlighted, also in view of the usage of these modelling tools for industrial purposes.

1. Introduction

Lithium-ion cells are employed in the vast majority of energy storage systems for hybrid and full electric vehicles, thanks to their high energy density, fast charging capabilities, and low self-discharge rate with respect to other battery types. Thermal management is a critical aspect of Li-ion battery packs as the cells can reach high temperatures during high current charge and discharge scenarios, reducing the battery lifespan and potentially leading to dangerous thermal runaway conditions. Several studies on the thermal management of Li-ion cells are available in the literature, based on both experimental and numerical techniques. Liu *et al.* [1] studied the change of internal characteristics of Li-ion cells with varying discharge rates using an experimental approach. Likewise, Keil and Jossen [2] assessed the impact of different charging strategies on the lifespan of 18650 cylindrical cells. Fan *et al.* [3] analysed the thermal management system of three air cooled battery packs, featuring aligned, staggered, and cross configurations, performing experiments in a small wind tunnel. Tan *et al.* [4] performed CFD analyses to study the effects of critical design and operational parameters on heat transfer performance in a liquid cooled battery module. Cao *et al.* [5] developed a Finite Element model of a battery pack cooled by an hybrid liquid-PCM system, validating their modelling approach

with experimental results. Li *et al.* [6] studied the thermal management of Li-ion cells by developing a 2D CFD model and a lumped parameter model and validated their results with wind tunnel measurements. Lebrouhi *et al.* [7] proposed a lumped parameter model to analyse continuous charging and discharging cycles of a battery pack with hybrid PCM-liquid cooling and validated their approach with both experimental and 3D CFD results. In all these studies, the availability of fast and reliable prediction tools emerges as a key concern.

This paper compares Computational Fluid Dynamics and lumped parameter modelling approaches to study the thermal management of Lithium-ion cells, using as a reference case one of the air-cooled battery pack configurations presented in the experimental study by Fan *et al.* [3]. The CFD model of the battery module and its cooling system is developed by modelling half of the physical domain exploiting the symmetry of geometry and flow, in an effort to reduce the required computational cost. The lumped parameter modelling approach is based on the use of the correlation by Zukauskas [8] for tube banks in cross flow, including the spacing-based correction factor proposed by Kim [9]. The overall heat transfer performance of the system is modelled by a single convective resistance, computed following the approach presented by Mahamud *et al.* [10]. Finally, numerical results on heat transfer from the CFD and reduced order models are compared with the experimental data presented by Fan *et al.* [3] to comparatively assess the accuracy of the proposed modelling approaches.

2. Materials and methods

2.1. Case study

This paper studies the thermal management of an air cooled battery pack which was originally examined by Fan *et al.* [3] using experimental methods. The battery module, represented in the schematic of figure 1a, is composed by thirty two Li-ion cylindrical cells arranged in a square lattice with spacing $S = 22$ mm. These are high energy density commercial 18650 cells, specifically the LG INR18650 model, as shown in figure 1b. The cells feature an external diameter of 18 mm and a height of 65 mm. Their nominal voltage is 3.635 V, while the nominal capacity is $C = 3.50$ Ah. The maximum internal impedance specified by the manufacturer is 40 m Ω . The battery module is placed within a 92x65 mm rectangular duct where a DC centrifugal fan is employed to cool the cells. The locations marked by the red dots in figure 1a correspond to the positions of the thermocouples used by Fan *et al.* [3], and the virtual probes included in the CFD model to compute the cell temperatures as in the experimental tests.

2.2. Computational Fluid Dynamics model

The CFD model of the presented battery pack and its cooling system is developed by using a two-dimensional approach, and modelling half of the physical domain, exploiting the symmetry of the geometry and flow with respect to the centreline of the air duct. The steady-state and incompressible flow solution is attained by numerically solving the RANS and energy equations.

$$\begin{cases} \nabla \cdot (\vec{u} \otimes \vec{u}) = -\frac{1}{\rho} \nabla p + \nabla \cdot [(\nu + \nu_t) \nabla \vec{u}] \\ \nabla \cdot \vec{u} = 0 \\ \nabla \cdot (T \vec{u}) = \nabla \cdot [(\alpha + \alpha_t) \nabla T] \end{cases} \quad (1)$$

The turbulent viscosity term ν_t in equations (1) is computed using the k - ω SST turbulence model [11] with a low-Reynolds wall modelling approach, as suggested in [9]. The thermal eddy diffusivity is obtained by introducing the turbulent Prandtl number, which is set to 0.85:

$$\alpha_t = \frac{\nu_t}{Pr_t} . \quad (2)$$

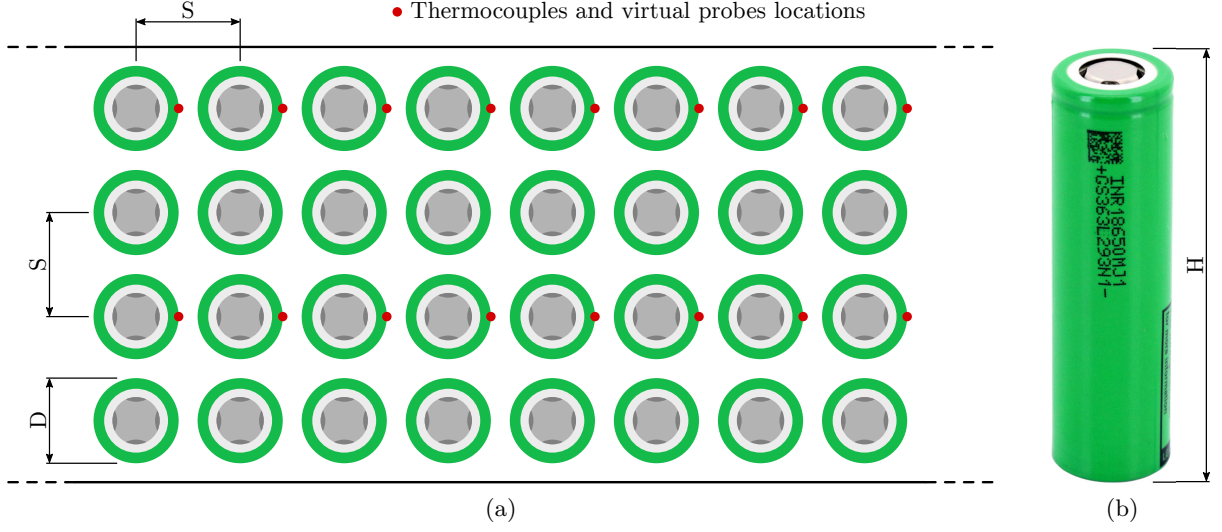


Figure 1. Cylindrical battery cells arranged in a square lattice, along with the relevant dimensional parameters (a), and a picture of a single commercial LG INR18650 cell (b).

The cooling air is modelled as an incompressible gas, its thermophysical properties are assumed uniform over the domain and constant with respect to pressure and temperature. The values of the thermophysical properties listed in table 1 are computed by means of the CoolProp library [12], considering a temperature of $T_{\text{ref}} = 20^\circ\text{C}$ and a barometric pressure of 101325 Pa.

At the inlet of the air duct the velocity field is set uniformly to u_{in} , which takes values of 0.6, 2.0, and 4.0 m/s in this analysis. The air inlet temperature is set to T_{ref} , while a zero gradient condition is assigned to the pressure field. The relative pressure over the outlet boundary is set to an arbitrary zero value, while zero gradient conditions are assigned to the velocity and temperature fields. Symmetry boundary conditions are applied to all fields at the surface corresponding to the symmetry plane of the channel. At the duct wall and the cells surface no-slip conditions are enforced, furthermore, the duct wall is assumed adiabatic. At the surface of each cell a uniform temperature gradient is imposed to obtain an entering heat flux:

$$\frac{\partial T}{\partial n} = \frac{\dot{Q}_g}{\pi D H \lambda} . \quad (3)$$

$\dot{Q}_g$ is the heat generated by a single cell, which is computed by considering the maximum internal impedance value $R_i = 40 \text{ m}\Omega$, and C-rate values of 0.5, 1.0, and 2.0 h^{-1} :

$$\dot{Q}_g = R_i I^2 = R_i (\text{C-rate} \times C)^2 . \quad (4)$$

Table 1. Values of the thermophysical properties of air, computed at the reference temperature $T_{\text{ref}} = 20^\circ\text{C}$ and pressure $p_{\text{ref}} = 101325 \text{ Pa}$.

Property	Symbol	Value	Units
Density	ρ	1.204	kg m^{-3}
Dynamic viscosity	μ	1.820×10^{-5}	$\text{kg m}^{-1} \text{s}^{-1}$
Thermal conductivity	λ	0.026	$\text{W m}^{-1} \text{K}^{-1}$
Specific heat	c_p	1006	$\text{J kg}^{-1} \text{K}^{-1}$

$\dot{Q}_g$ is obtained by considering just the contribution of Joule heating, and neglecting the effects of entropy changes, i.e. the second term of Bernardi's equation [13], resulting from chemical reactions occurring during charging and discharging operations. Considering these effects would require modelling the internals of each cell, thus increasing the model complexity and computational cost. Besides, obtaining accurate estimates of entropy effects is not a trivial task, as data in the literature is scarce. The governing equations are discretised by means of a staggered Finite Volume approach, addressing the pressure-velocity coupling by a variant of the SIMPLE algorithm [14], which is implemented in the OpenFOAM computational toolkit [15]. Second-order accurate upwind schemes are used for advective terms, while diffusive terms are handled with central schemes with explicit non-orthogonality corrections. The physical domain is subdivided in cells using an advancing front algorithm. Figure 2 shows the resulting computational domain which features extended inlet and outlet sections to allow for proper flow development; in addition, figure 2 presents a detailed view of a section of the grid which includes two battery cells, the symmetry plane on the left, and the duct wall on the right.

2.3. Grid sensitivity analysis

The influence of the grid on numerical results is assessed by developing three computational meshes with different cell sizes, and comparing numerical results obtained at $u_{in} = 4.0$ m/s and C-rate = 1 h⁻¹. These are expressed as the maximum temperature difference between the battery cells and the air flow entering the duct:

$$\Delta T_m = \max(T_i - T_{ref}) , \quad (5)$$

where the subscript i identifies each of the virtual temperatures probes present in the schematic of figure 1a. The coarse and fine computational meshes are obtained by doubling and halving the size of the first near-wall element of the medium mesh, respectively, while maintaining the same size ratio with the far-field elements of approximately 27.5. Numerical results from the three computational grids are listed in table 2, along with the size of the first elements along the wall normal direction Δ_w , the integral mean values of the dimensionless wall distance y^+ , and the ΔT_m value obtained at zero grid spacing by means of Richardson's extrapolation. As the element size decreases, numerical results tend to converge rapidly, with a 1.5% deviation between the fine and medium grids. The mean y^+ values are below unity in all cases which is consistent with selected near-wall modelling approach. Both the medium and fine grids produce results close to the theoretically exact solution, showing deviations of 2.0% and 0.5%, respectively. The following CFD analyses are performed on the basis of the medium mesh, since the discretisation error with respect to the fine mesh and the exact solution are acceptable when considering the substantial savings in terms of computational cost.

Table 2. Numerical results obtained from the coarse, medium, and fine computational grids, along with the exact solution from Richardson's extrapolation.

	Δ_w [mm]	$\bar{y}^+$	ΔT_m	Difference to previous grid
Coarse grid	0.016	0.425	2.987	-
Medium grid	0.008	0.120	3.256	8.98%
Fine grid	0.004	0.105	3.306	1.53%
Richardson's extrapolation	0.0	0.0	3.322	0.50%

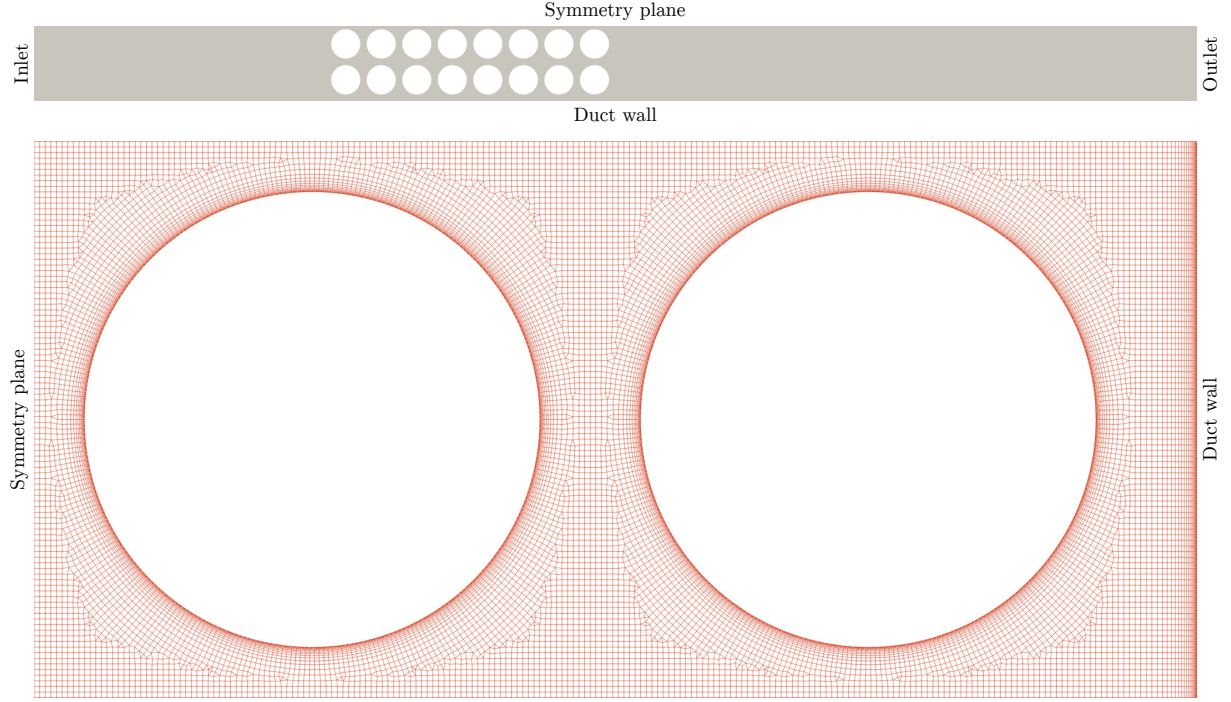


Figure 2. Overall view of the computational domain including sixteen cells and half of the cooling duct, and a detailed view of a section of the grid which includes two battery cells, the symmetry plane, and the duct wall.

2.4. Reduced order model

Under the assumptions of steady-state conditions and isothermal cells, the electro-thermal analogy applied to the whole battery pack reads:

$$\bar{T}_{\text{cell}} - \bar{T}_{\text{air}} = \dot{Q}_{\text{tot}} R_{\text{conv}} , \quad (6)$$

where $\bar{T}_{\text{cell}}$ represents the average cell surface temperature, while $\bar{T}_{\text{air}}$ is the average air temperature between the inlet and outlet of the duct. $\dot{Q}_{\text{tot}} = 32 \dot{Q}_{\text{g}}$ is the total heat generated in the pack and R_{conv} is the equivalent convective thermal resistance between the airflow and the cells. R_{conv} is computed by following the approach proposed by Mahamud *et al.* [10]:

$$R_{\text{conv}} = \frac{1}{\dot{m} c_p (1 - e^{-\text{NTU}})} , \quad \text{NTU} = \frac{32 \pi \lambda H}{\dot{m} c_p} \text{Nu} (1.0 - 2.26 e^{-1.675 S}) , \quad (7)$$

where the value of the Nusselt number Nu is obtained from the correlation proposed by Zukauskas [8] for tube banks in cross flow; Nu is then multiplied by the correction factor proposed by Kim [9] in equation (7).

$$\text{Nu} = \varepsilon_n 0.27 \text{Re}_{\text{max}}^{0.63} \text{Pr}^{0.36} (\text{Pr}/\text{Pr}_w)^{0.25} \quad \text{for} \quad 10^3 < \text{Re}_{\text{max}} < 2 \times 10^5 \quad (8)$$

In the equation above Re_{max} is the Reynolds number value computed by considering the fluid velocity value in the gap between two adjacent cells. The latter, U_{max} , is simply obtained by applying mass conservation. In equation (8) Pr stands for the value of the Prandtl number evaluated at the average air temperature $\bar{T}_{\text{air}}$, while Pr_w is computed at the mean cell temperature $\bar{T}_{\text{cell}}$. The correction factor ε_n depends on the number of cell columns and it is obtained from the values listed in table 3.

3. Results

3.1. CFD results

Figure 3 shows velocity magnitude and temperature increase colour maps, each made on half of the physical domain. As the flow approaches the first column of cells fluid velocity sharply increases as air enters the interstitial space between cells; these high velocity streams flow through the pack undisturbed by the successive cells, thus leaving behind regions of stagnating flow between the front and backward facing portions of the cells surface, thus diminishing the local heat transfer effectiveness. At the battery pack outlet, the two streams near the centreline merge together, while the one close to the wall adheres to it, forming a large wake behind the last column of cells. As previously anticipated, the cells hot-spots are located in correspondence of the stagnating fluid regions, while the zones lapped by the high velocity streams feature far lower temperature increase values. The accuracy of the proposed CFD methodology is assessed by comparing the maximum temperature rise values obtained numerically at the virtual probes locations in figure 1a with their experimental counterparts, as shown in figure 4a. Overall, numerical results are in good agreement with the experimental data for most of the C-rate and u_{in} configurations considered in [3], apart from a couple of outliers at $u_{\text{in}} = 0.6$ m/s. Besides other sources of uncertainty, such as variations of the internal impedance of the cells or the positioning of the thermocouples in the reference experiment, these large discrepancies and, in particular, the overestimation of the maximum temperatures for the cases at $u_{\text{in}} = 0.6$ m/s, can be linked to the prediction of flow features in the wake of the cells. The dimensionless velocity contours in figure 4b highlight that, for $u_{\text{in}} = 0.6$ m/s, a vast stagnation zone is predicted by the CFD model, whereas a secondary flow component is detected for the other flow rates. This behaviour could be associated with the use of a RANS turbulence model which, by its nature, tends to average out large scale oscillations which could actually occur in the real-world case. On average, numerical results at 0.5C underestimate their experimental counterparts with greater margins with respect to the other cases. This might be a result of neglecting the contribution of entropy changes to the generated heat, which become particularly relevant at low C-rates. At $u_{\text{in}} = 0.6$ m/s and C-rate = 0.5 h^{-1} the aforementioned uncertainty sources seem to compensate each other leading to a very good agreement. Nevertheless, the proposed CFD approach showed remarkable accuracy, especially considering that the physical problem at hand is modelled as a 2D steady state problem, whereas it is a 3D and transient problem, not only due to the time-dependent features typical of flows around cylinders, but also because cell properties change over time with the decreasing state of charge.

3.2. Lumped parameter model results

Figure 5 shows the comparison between the temperature increase values obtained from the lumped parameter model ΔT_{LPTN} , the mean values obtained experimentally $\Delta T_{\text{a exp}}$, and those obtained from the mean of the CFD derived integral average cell temperature values $\Delta T_{\text{a CFD}}$. When compared with the experimental data ΔT_{LPTN} values represent a substantial underestimate; this is expected since empirical correlations, like the one by Zukauskas [8], are based on the mean temperature of a given surface, not on the hot-spot temperature which was measured in [3]. If the CFD model described in §2.2 can be considered as a reliable prediction

Table 3. Values of the correction factor ε_n as a function of the number of cell columns.

Number of columns	1	2	3	4	5	6	7	8	9
ε_n	0.700	0.800	0.865	0.910	0.928	0.942	0.954	0.965	0.972

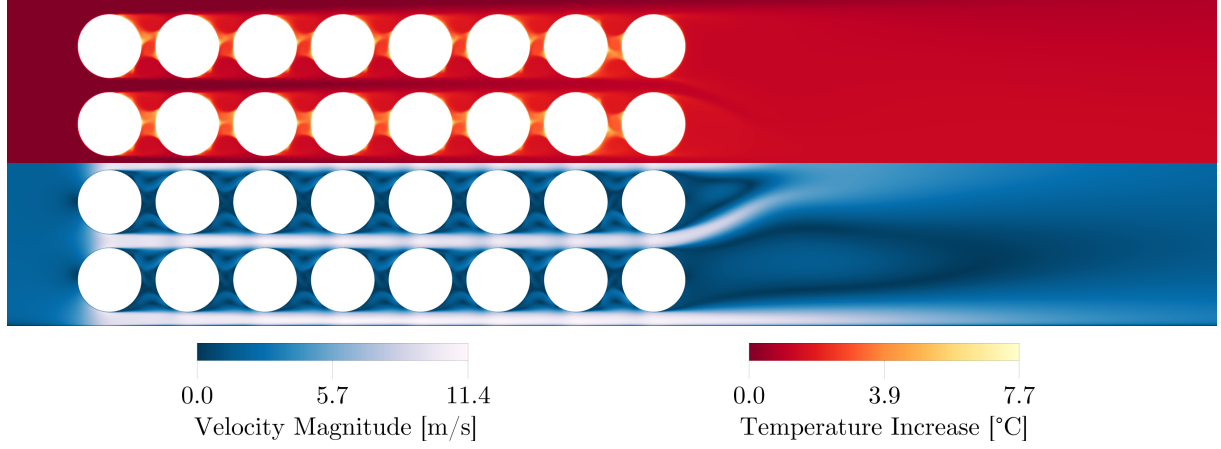


Figure 3. Colour maps of air velocity magnitude and temperature increase, considering 2 m/s inlet air velocity and unitary C-rate.

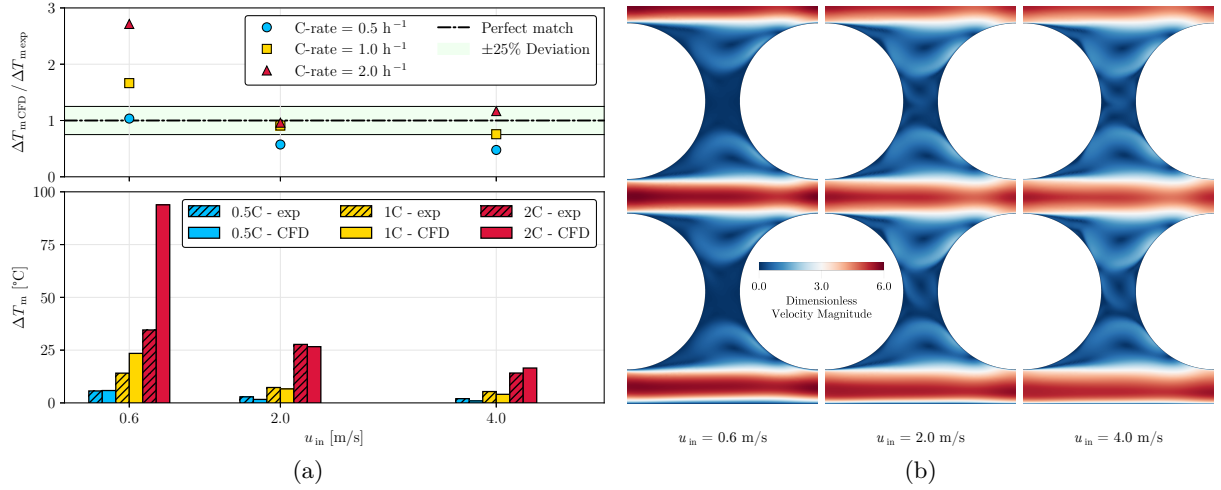


Figure 4. Comparison between numerical and experimental values of maximum temperature increase ΔT_m (a) associated with the virtual probes and thermocouples seen in figure 1a, and colour maps of dimensionless velocity magnitude (b).

tool, then the lumped parameter model represents a quick and simple approach for obtaining fair estimates about the overall behaviour of the cooling system, given the reasonable accuracy levels seen in figure 5b.

4. Concluding remarks

This paper presented the development and comparison of CFD and lumped parameter modelling approaches, to study the thermal management of a Li-ion battery pack which was the focus of an experimental study available in the literature. The CFD model was developed by using a two-dimensional approach and exploiting the symmetry of the examined problem, while the lumped parameter approach was formulated on the basis of empirical correlations available in the literature. Numerical results obtained with both approaches were compared with the available experimental data and between each other. Overall, the proposed CFD methodology showed remarkable accuracy levels in the high inlet velocity cases, while it failed to capture secondary flows in the cells wakes at the lowest inlet velocity value considered, thus leading

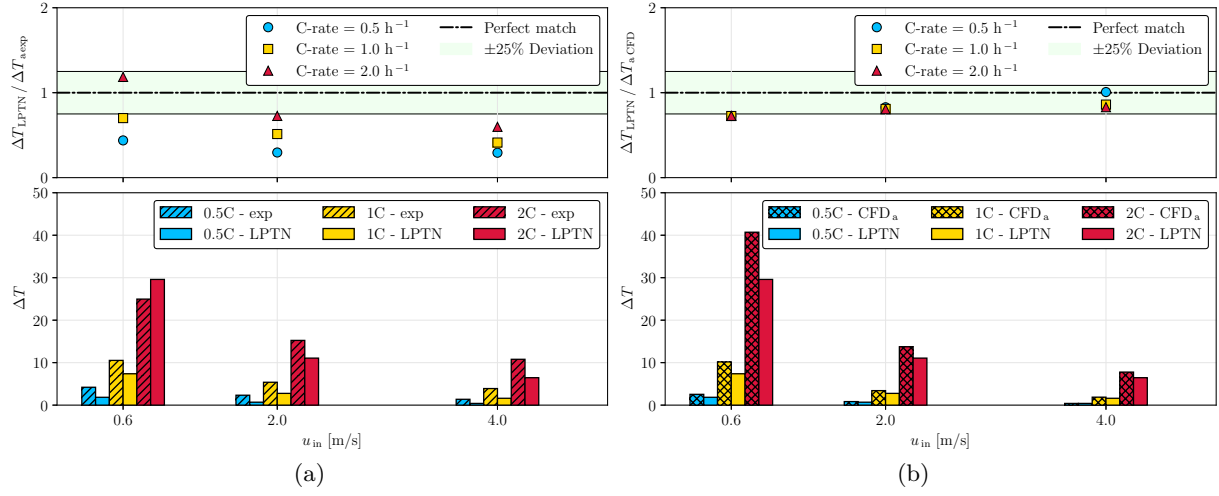


Figure 5. Comparison between the temperature increase values obtained from the reduced order model ΔT_{LPTN} and those obtained experimentally ΔT_{aexp} (a), and from the mean of the CFD derived average cell temperatures ΔT_{aCFD} (b).

to great overestimates of the cell temperatures. The developed lumped parameter approach underestimated the experimental temperature increase values, however, the reasonable accuracy levels noted in the comparison with CFD results suggests that the reduced order model can be considered as a simple and fast method to derive fair estimates about the average performance of the overall system. On the other hand, the CFD and experimental approaches are required when seeking accurate hot spot temperature figures. Anyway, the developed CFD model only requires a moderate computational effort, making it a viable alternative to expensive and time consuming experimental tests. Future research efforts will be aimed at improving both the CFD and reduced order approaches by including a detailed model of the cell internals. In addition, the developed methodologies will be applied to other battery pack configurations.

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