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INTRODUCTION

Lithium batteries have made substantial and significant gains in the last 30 years from becoming a curiosity to becoming the dominant rechargeable battery for consumer portable applications. However, the next market opportunities will be much tougher to conquer as they mostly demand higher power capabilities at lower costs.

A detailed study of one commercial Li-ion Polymer battery (EEMB. LP703048. 1000 mAh)¹, taking into account mainly its electrical behaviour, has been considered.

No.	Item	Characteristics	Remark	No.	Item	Criteria	Test Instructions
2.1	Model	LP703048		5.1.1	1C ₅ A rate discharge capacity	Discharge Time ≥ 57min	Full charge at 20 ± 5 °C, rest for an hour, then discharge at the same temperature with 1.0C ₅ A to 2.75V
2.2	Capacity	Nominal Capacity	1000 mAh	0.2CA	5.1.2	High temp. discharge capacity	Discharge Time ≥ 54min
		Minimum	950 mAh	0.2CA			
2.3	Nominal Voltage	3.7 V		5.1.3	Low temp. discharge capacity	Discharge Time ≥ 4.25h	Full charge at 20 ± 5 °C, store at 55 ± 2 °C for 16h-24h, then discharge at the same temperature with 1.0C ₅ A to 2.75 V
2.4	Weight	Approx. 20 g					
2.5	Internal Impedance	≤ 100	mΩ	AC 1KHz (50%前電)	5.1.4	Cycle Life	≥ 300Cycles
		Length	≤ 4.9	mm			
		Width	≤ 30.5	mm			
2.6	Dimension	Thickness	≤ 7.3	mm	5.1.5	Capacity Retention	Discharge Time ≥ 4.5 h
		Maximum Current	1000	mA			
2.7	Charge	Limited Voltage	4.200 ± 0.020	V			
		End of Current	20	mA			
2.8	Discharge	Maximum Current	2000	mA			
		End Voltage	2.75 ± 0.005	V			
2.9	Operation Temperature	Charge	0 ~ +45	°C			
		Discharge	-20 ~ +60	°C			
		1 month	-20 ~ +60	°C			
2.10	Storage Temperature	3 month	-20 ~ +45	°C			
		12 month	-20 ~ +25	°C			
2.11	Storage Relative Humidity	65 ± 20	%				

Figure 1. Electrical Characteristics: Li-Ion Polymer Battery (EEMB. LP703048. 1Ah).

COMPUTATIONAL METHODS

With a view to estimating electrical characteristics of a Polymer Li-ion Battery during specific charge and discharge conditions, a **COMSOL Multiphysics®** model has been developed that accounts for electrochemical phenomena inside the device. In order to accomplish that, the **Battery and Fuel Cells Module** has been used. Cell model has been created using the Li-Ion Battery interface, customizing material properties and electrochemical reactions. The electrochemical parameters required for the calculation have been determined by laboratory tests, manufacturer datasheets and literature survey.

A detailed analysis has been performed to evaluate the influence of the electrode kinetics in the characteristic curve of the device³. As shown in **Figure 2**, the Lithium Insertion electrode kinetics is the most accurate approximation to the device experimental behaviour.

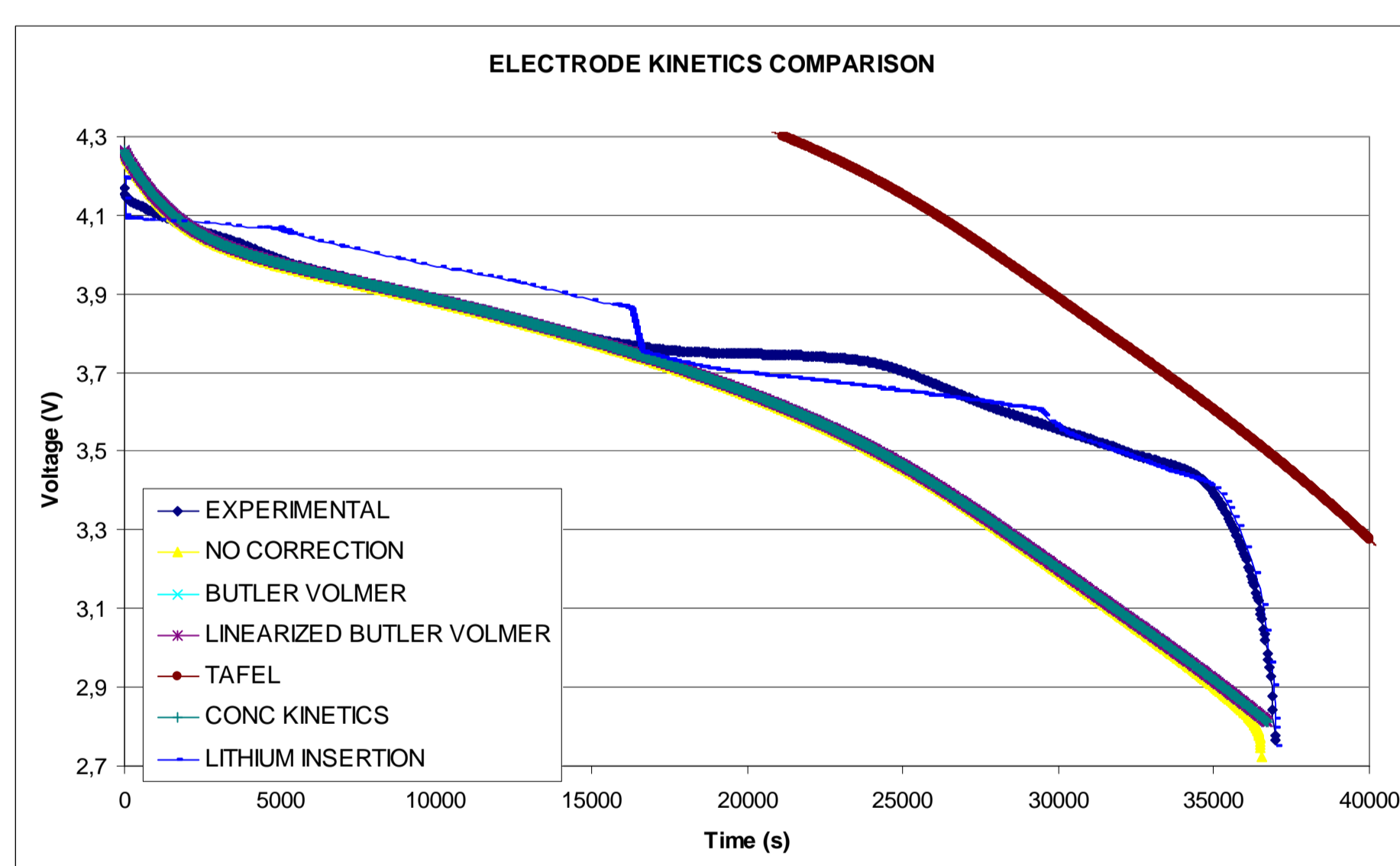


Figure 2. Electrode kinetics comparison.

The equilibrium potential of the Li-ion intercalation electrodes does not follow the Nerst equation due to the solid state redox reaction². The effect of the equilibrium potential correction fitted in the **COMSOL Multiphysics®** model was studied for different discharge rates. As a result, the Redlich-Kister equation for LiC₆ and LiCoO₂ was used. **Table 1 and 2** show the equations used for equilibrium potential calculation and the parameters values used, respectively⁴.

Table 1. Model equations for equilibrium potential using various equations of state.⁴

Model equations for equilibrium potential using various equations of state	
One parameter Margules	$FU = FU^0 + RT \ln \left(\frac{1-x_2}{x_2} \right) + RT [A(2x_2 - 1)]$
Two parameter Margules	$FU = FU^0 + RT \ln \left(\frac{1-x_2}{x_2} \right) + RT [-A_0 + 2A_1x_2 - B_0 + 3B_1x_2 - \frac{1}{2}B_2x_2^2]$
van Laar equation	$FU = FU^0 + RT \ln \left(\frac{1-x_2}{x_2} \right) + RT \left[\frac{A_1x_2^2 + 2A_2x_2 - A_3}{1-x_2 + A_4x_2^2} \right]$
Redlich-Kister expansion	$FU = FU^0 + RT \ln \left(\frac{1-x_2}{x_2} \right) + \left\{ \sum_{k=0}^N A_k \left[(2x_2 - 1)^{k+1} - \frac{2x_2(1-x_2)}{(2x_2 - 1)^{k+2}} \right] \right\}$

Table 2. Parameter values using Redlich-Kister equation for LiC₆ and LiCoO₂.⁴

Parameters	MCMB	LiCoO ₂
N	10	7
U ₀	-1.7203 ± 0.51308	-29.614 ± 2.3806
A ₀	-0.35799 × 10 ⁶ ± 0.99032 × 10 ⁶	0.64832 × 10 ⁶ ± 0.45034 × 10 ⁶
A ₁	-0.35008 × 10 ⁶ ± 0.99055 × 10 ⁶	-0.65173 × 10 ⁶ ± 0.45933 × 10 ⁶
A ₂	-0.35247 × 10 ⁶ ± 0.98397 × 10 ⁶	0.65664 × 10 ⁶ ± 0.45969 × 10 ⁶
A ₃	-0.35692 × 10 ⁶ ± 0.97652 × 10 ⁶	-0.65787 × 10 ⁶ ± 0.46137 × 10 ⁶
A ₄	-0.38633 × 10 ⁶ ± 0.10929 × 10 ⁶	0.63021 × 10 ⁶ ± 0.44922 × 10 ⁶
A ₅	-0.35908 × 10 ⁶ ± 0.11797 × 10 ⁶	-0.59465 × 10 ⁶ ± 0.37283 × 10 ⁶
A ₆	-0.28794 × 10 ⁶ ± 0.52429 × 10 ⁶	0.27113 × 10 ⁶ ± 0.21054 × 10 ⁶
A ₇	-0.14979 × 10 ⁶ ± 0.80161 × 10 ⁶	-0.69045 × 10 ⁶ ± 0.56136 × 10 ⁶
A ₈	-0.39912 × 10 ⁶ ± 0.20291 × 10 ⁶	
A ₉	-0.96172 × 10 ⁶ ± 0.31894 × 10 ⁶	
A ₁₀	-0.63262 × 10 ⁶ ± 0.14748 × 10 ⁶	

The model has been verified by voltage/ amperage measurements by means of a commercial Battery Testing System (CADEX C8000). These tests have provided a more realistic approach of electrochemical mechanisms inside the device.

RESULTS

Because of validation purposes both, an experimental (CADEX C8000) and a theoretical analysis (COMSOL model) reproducing datasheet test instructions, had been carried out. **Figure 3** shows the 1C₅A rate discharge capacity test results.

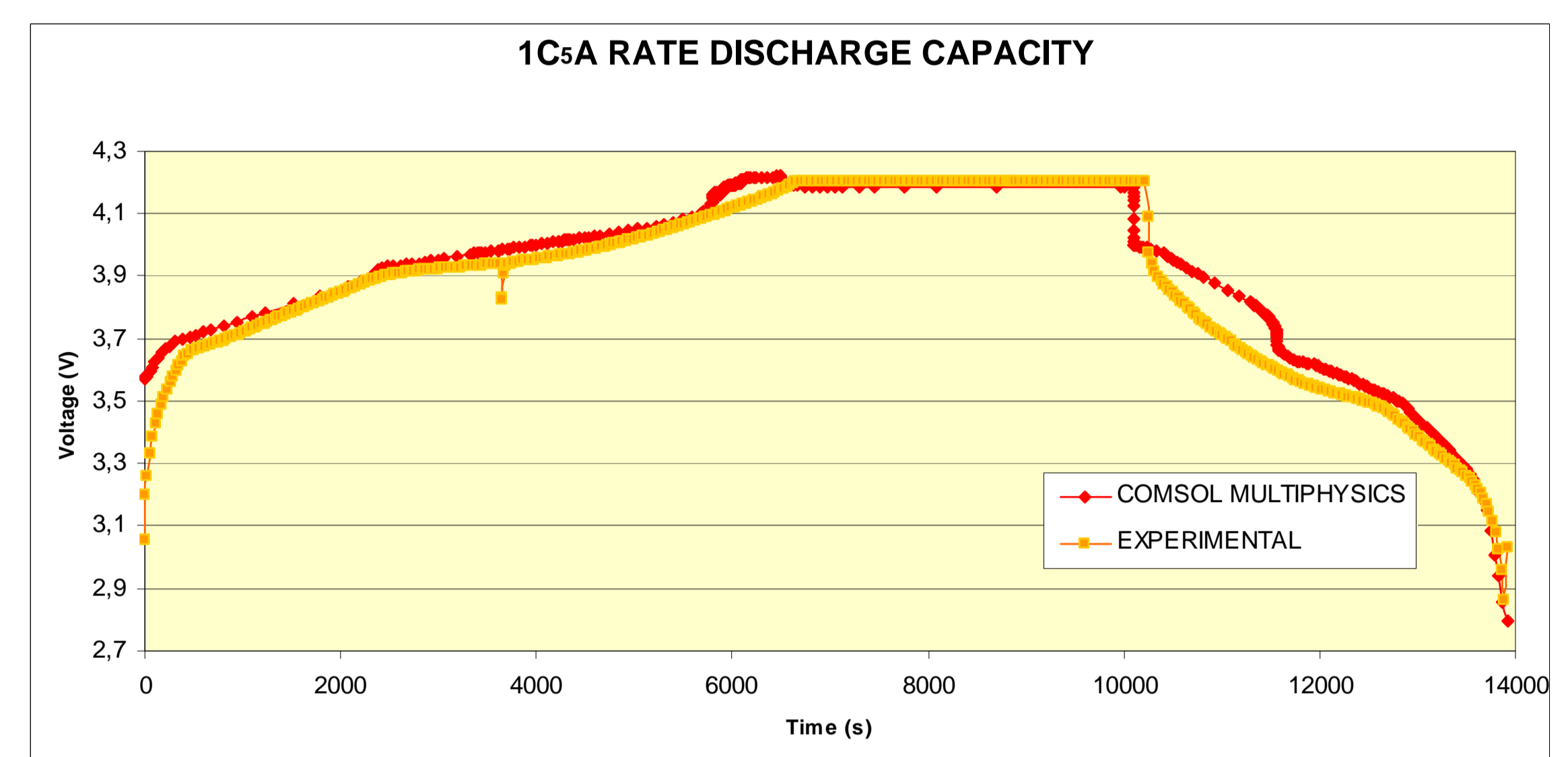


Figure 3. 1C₅A rate discharge capacity.

In both cases very similar results are achieved. Some of the differences might be due to differences in the state of charge considered in the theoretical model, intrinsic electrochemical parameters of the battery and/or geometrical aspects entered in the model (electrode/separator length, cell area,...)

Figure 4 shows some battery characteristic curves at different discharge rates predicted by the **COMSOL Multiphysics®** model.

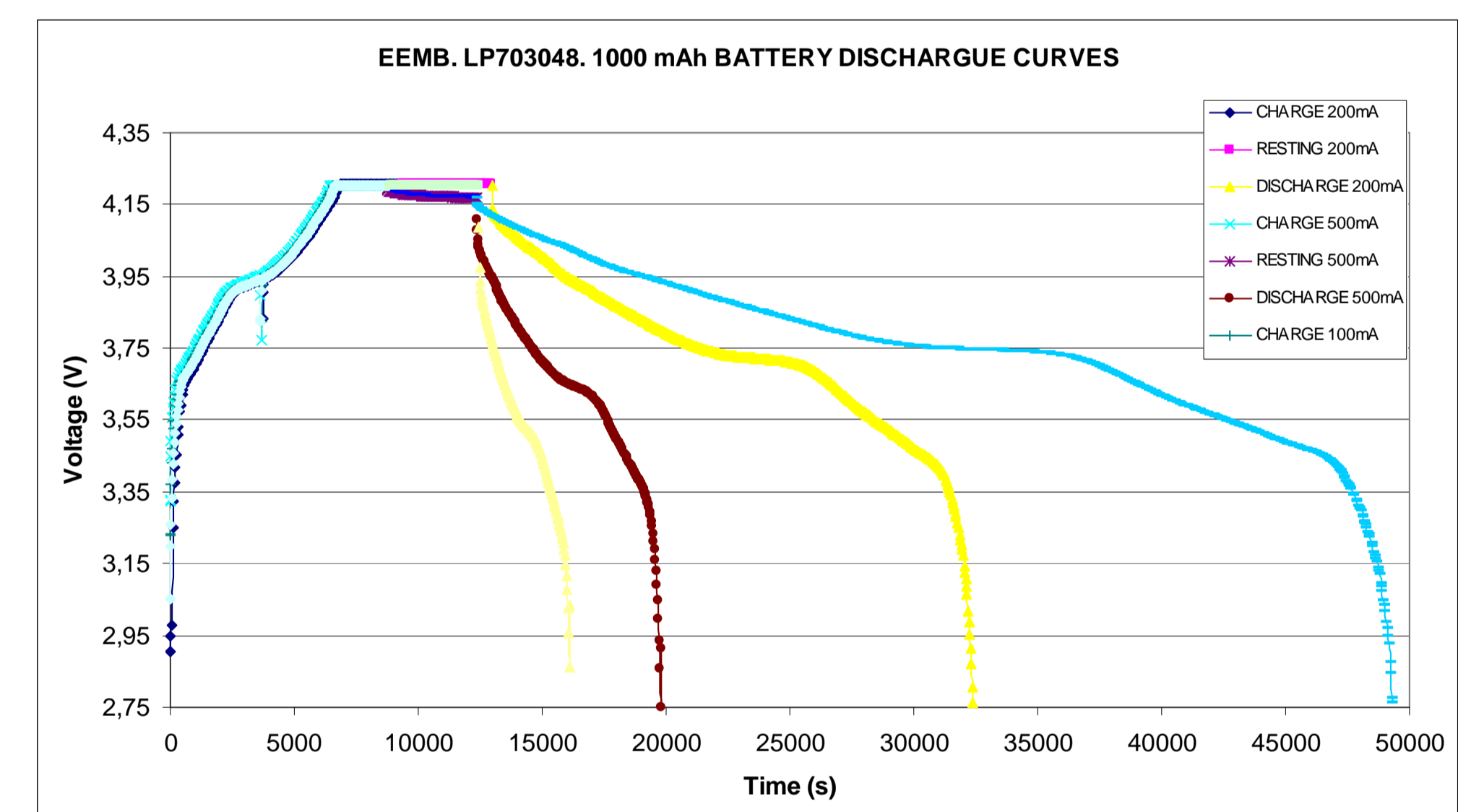


Figure 4. Characteristic curves at different discharge rates.

CONCLUSIONS

Results indicate that **COMSOL Multiphysics®** model is able to predict accurately not only the electrical behaviour of the device under specific operating conditions but also the influence of the materials involved, geometric aspects and other relevant boundary conditions in battery performance.

REFERENCES

1. M. Cai, T. Cheng, A. Lee. EEMB CO., LTD Polymer Li-ion Battery Specification.
2. N.Yabuuchi, Y.Makimura, T. Ohzuku. J. Electrochemical Society. 154 (2007) 1314-A321.
3. L.Gao, S.Liu, R.A. Dougal. Dynamic Lithium-Ion Battery Model for System Simulation. IEEE Transactions on Components and Packaging Tech. Vol. 25, No. 3, Sept. 2002.
4. D. K. Karthikeyan, G. Sikha, R. E. White. Thermodynamic model development for Li intercalation electrodes. Journal of Power Sources 185 (2008) 1398-1407