

Supporting information for

Gas Phase Composition of a NiMH during a work cycle

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MS calibration sampler

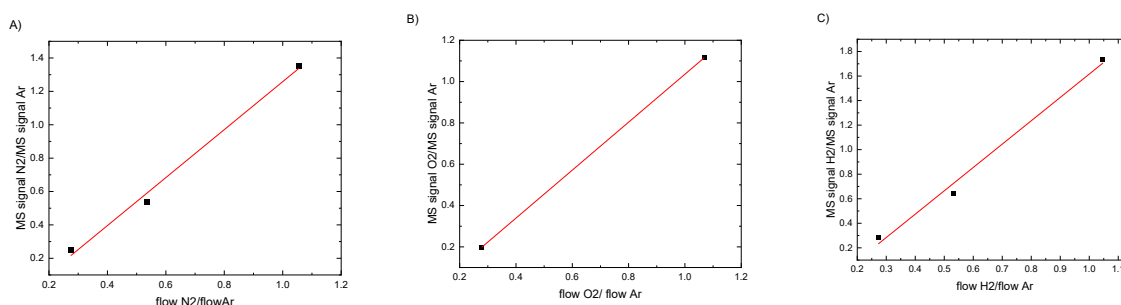


Figure S1. The calibration curves for A) nitrogen, B) oxygen and C) hydrogen, normalized by argon signal.

Table S1. Flow rates of the calibration gasses individually mixed with Ar

Gas/ Flow (ml min ⁻¹)	N ₂	H ₂	O ₂	Ar
	20.6	20.5	20.9	19.1
	11.1	11.0	11.3	19.1
	6.4	6.3	6.5	19.1

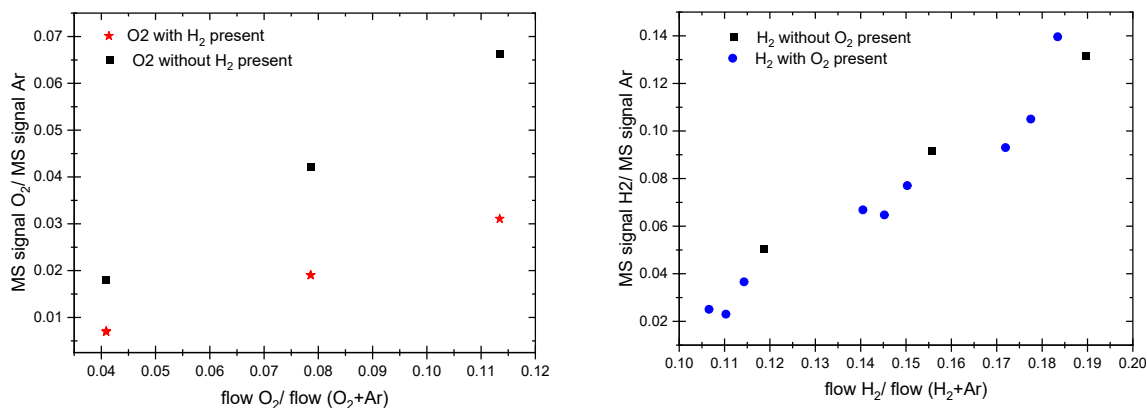


Figure S2. MS calibration curve obtained with O₂ and H₂ mixture, with 20 ml min⁻¹ Ar flow, as a

carrier gas.

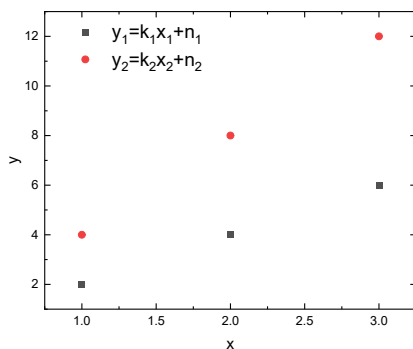


Figure S3. General example of the situation given in the Figure S2.

Figure S3 presents general case showing two data sets, similar to the Figure S2 A). To correct for this deviation y_2 can be calculated as:

$$y_2 = k_2 \left(\frac{y_1 - n_1}{k_1} \right) + n_2$$

Real oxygen signal is in that case:

$$O_2 = \frac{\frac{O_2}{Ar} + n_2}{k_1 * k_2 - n_1}$$

And water:

$$H_2O = \frac{H_2O}{Ar} - \left(k * \frac{O_2}{Ar} + n \right)$$

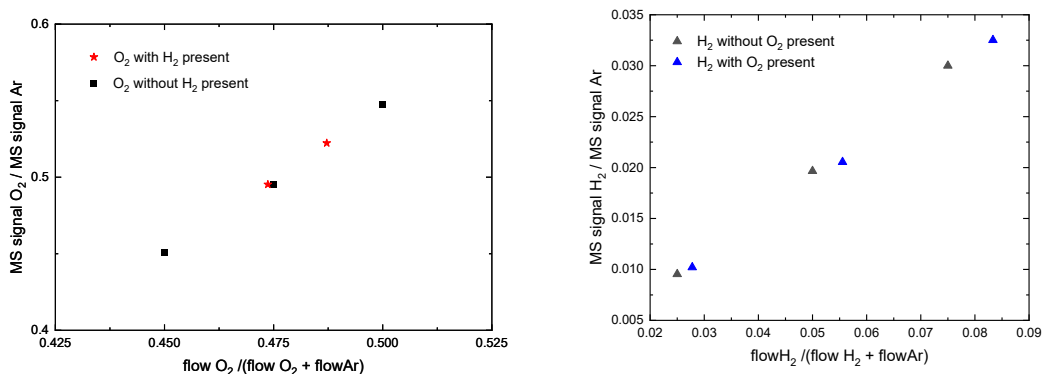


Figure S4. MS response when measuring O₂ and H₂ mixture, with Ar as a carrier gas

MS calibration microcapillary

For either H₂ or O₂ with N₂ calibration was performed by using two mass flow controllers and sampling the stream. A backpressure regulator was used to investigate if the pressure affected the signal. For all measurements a total flow of 200 ml/min was used.

O₂ with N₂ calibration

As can be seen in Figure S5 the MS signal follows the set dilution well. When the total pressure is increased the total signals for both O₂ and N₂ were increased. However, the proportion of the two signals remained constant.

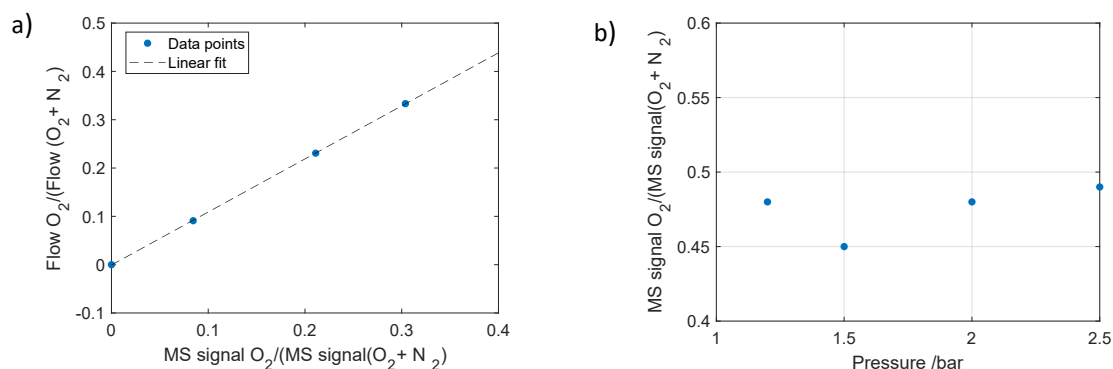


Figure S5. a) MS calibration curve obtained with O₂ and N₂ mixture at atm. (b) Raw MS signals compared at various total pressures. The set flow was 100 ml/min O₂ and 100 ml/min N₂.

H₂ with N₂ calibration

For H₂ with N₂ linear increases with dilution were obtained. However, as the pressure was increased the obtained ratio changed. As such, a different type of calibration was required. Considering how the signal for the same dilution changed with pressure the following function was utilized:

$$f(p_{abs}) = \frac{k_1}{(1 + e^{-k_2 * p_{abs}})^{k_3}} + k_4$$

Where k are constants and p_{abs} is the absolute pressure of the system.

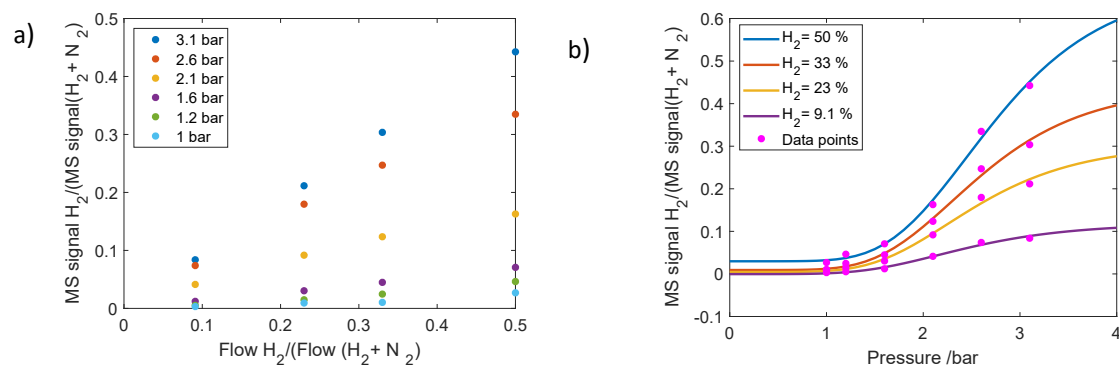


Figure S6. MS calibration curve obtained with H₂ and N₂ mixtures. A) MS signals compared to the set composition. B) MS signals for different gas compositions at various total pressures.

Using these empirical functions a calibration curve is made for each measured point and converted to the percentage.

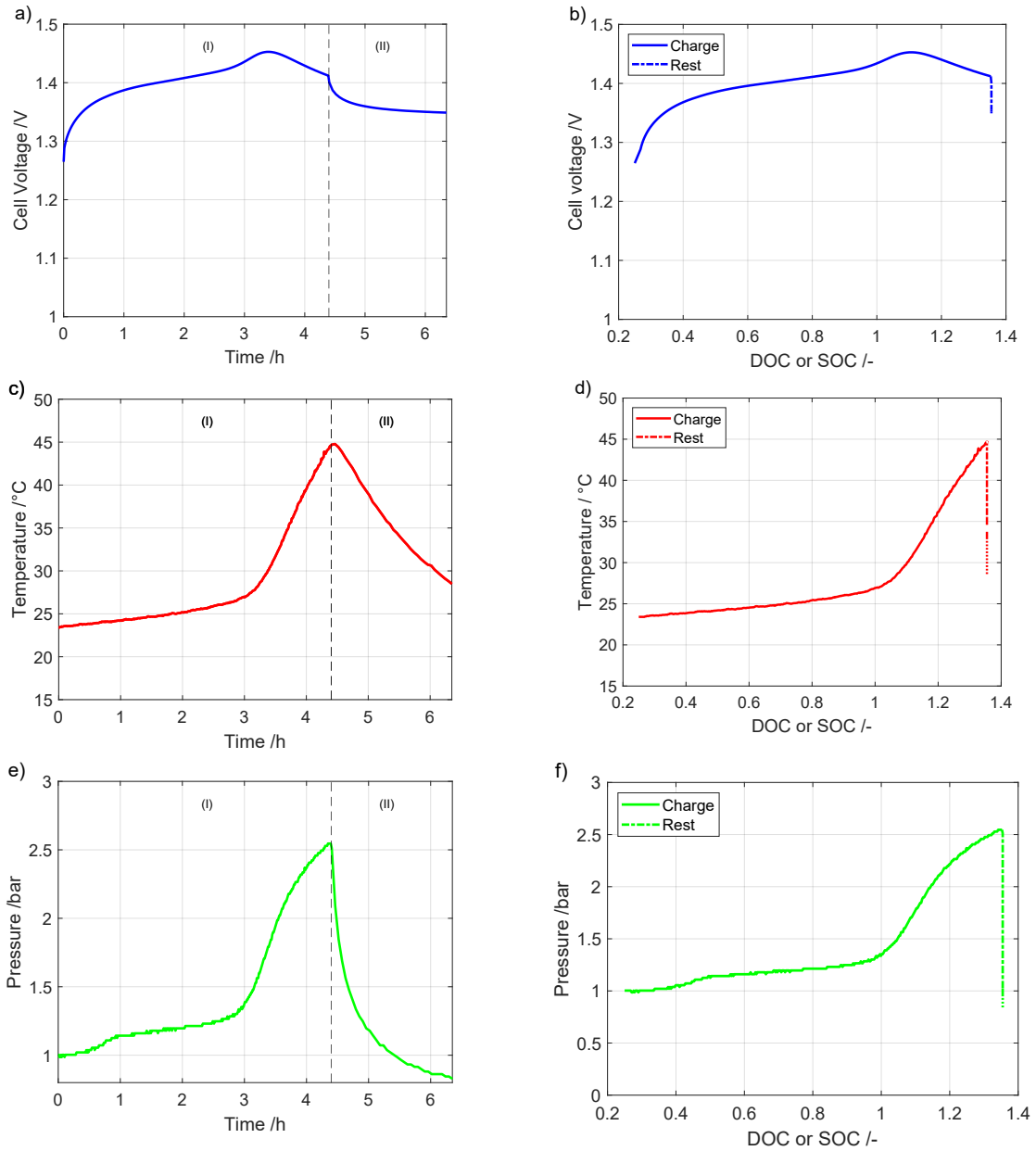


Figure S7. Cell voltage (a,b)/ temperature (c,d) and pressure (e,f) during overcharging the battery modul vs time (a,c,e) and DOC or SOC (b,d,f)