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In [23]: #0. Import all required modules
import pandas as pd
import pybamm
import numpy as np
import matplotlib.pyplot as plt
import glob
import os
```

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In [3]: os.chdir('C:/modelling/CN_cells_C50_GITT/')
```

```
In [5]: model = pybamm.lithium_ion.MSMR({"number of MSMR reactions": ('6', '4')})
param = model.default_parameter_values
solution = []
```

```
In [7]: U0 = [0.07833993326963097, 0.08636841987406249, 0.11390863812772753, 0.15930077772220294, 0.1987760913502005, 0.3148322232851191]
X0 = [0.320811403373459, 0.23525018228639896, 0.23857806885205055, 0.10092783640161686, 0.04283677507564162, 0.06083044471042518]
W0 = [0.03955880194055436, 0.925732506079815, 0.05808806812311207, 0.7260732959764035, 0.11169328422750696, 4.150274910982206]
```

```
In [9]: #MSMR parameter update
for i in range(0,6):
    param.update(
        {
            f'U0_n_{i}': U0[i], f'X0_n_{i}': X0[i], f'W0_n_{i}': W0[i],
            #'a_n_0': 0.5, 'a_n_1': 0.5, 'a_n_2': 0.5, 'a_n_3': 0.5, 'a_n_4': 0.5, 'a_n_5': 0.5,
            #'j0_ref_n_0': 2.7, 'j0_ref_n_1': 2.7, 'j0_ref_n_2': 2.7, 'j0_ref_n_3': 2.7, 'j0_ref_n_4': 2.7, 'j0_ref_n_5': 2.7,
        }, check_already_exists=False
    )
```

```
In [21]: pybamm.set_logging_level('INFO')

experiment = pybamm.Experiment(
    [(
        "Discharge at C/3 for 20 hours or until 2.8 V",
        "Charge at C/3 until 4.20 V",
    )]*2,
    period="10 seconds",
)
solver = pybamm.CasadiSolver(mode="safe", return_solution_if_failed_early = True)
sim = pybamm.Simulation(model, experiment = experiment, parameter_values=param, solver = solver)
sol = sim.solve(calc_esoh=False)
solution.append(sol)
```

```
2024-08-21 17:14:43.147 - [INFO] callbacks.on_experiment_start(162): Start running experiment
2024-08-21 17:14:43.148 - [INFO] parameter_values.process_model(440): Start setting parameters for MSMR
2024-08-21 17:14:43.254 - [INFO] parameter_values.process_model(509): Finish setting parameters for MSMR
2024-08-21 17:14:43.255 - [INFO] parameter_values.process_model(440): Start setting parameters for MSMR
2024-08-21 17:14:43.328 - [INFO] parameter_values.process_model(509): Finish setting parameters for MSMR
2024-08-21 17:14:43.328 - [INFO] discretisation.process_model(149): Start discretising MSMR
2024-08-21 17:14:44.055 - [INFO] discretisation.process_model(251): Finish discretising MSMR
2024-08-21 17:14:44.055 - [INFO] discretisation.process_model(149): Start discretising MSMR
2024-08-21 17:14:45.014 - [INFO] discretisation.process_model(251): Finish discretising MSMR
2024-08-21 17:14:45.016 - [NOTICE] logger.func(7): Cycle 1/2 (35.100 us elapsed) -----
2024-08-21 17:14:45.017 - [NOTICE] logger.func(7): Cycle 1/2, step 1/2: Discharge at C/3 for 20 hours or until 2.8 V
2024-08-21 17:14:45.022 - [INFO] base_solver.set_up(117): Start solver set-up
2024-08-21 17:14:45.177 - [INFO] base_solver.set_up(286): Finish solver set-up
At t = 489.65 and h = 5.91765e-06, the corrector convergence failed repeatedly or with |h| = hmin.
At t = 218.229 and h = 5.16621e-06, the corrector convergence failed repeatedly or with |h| = hmin.
At t = 135.579 and h = 4.21644e-06, the corrector convergence failed repeatedly or with |h| = hmin.
At t = 64.6713 and h = 5.08181e-06, the corrector convergence failed repeatedly or with |h| = hmin.
The residual routine or the linear setup or solve routine had a recoverable error, but IDACalcIC was unable to recover.
The residual routine or the linear setup or solve routine had a recoverable error, but IDACalcIC was unable to recover.
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2024-08-21 17:14:49.817 - [NOTICE] logger.func(7): Cycle 1/2, step 2/2: Charge at C/3 until 4.20 V
2024-08-21 17:14:49.833 - [INFO] base_solver.set_up(117): Start solver set-up
2024-08-21 17:14:49.970 - [INFO] base_solver.set_up(286): Finish solver set-up
The residual routine or the linear setup or solve routine had a recoverable error, but IDACalcIC was unable to recover.
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2024-08-21 17:14:50.139 - [ERROR] callbacks.on_experiment_error(233): Simulation error: Maximum number of decreased steps occurred at t=122
20.000000001 (final SolverError: 'Error in Function::call for 'F' [IdasInterface] at ../casadi/core/function.cpp:1432:
Error in Function::call for 'F' [IdasInterface] at ../casadi/core/function.cpp:361:
../casadi/interfaces/sundials/idas_interface.cpp:596: IDACalcIC returned "IDA_NO_RECOVERY". Consult IDAS documentation.'). For a full solu
tion try reducing dt_max (currently, dt_max=600) and/or reducing the size of the time steps or period of the experiment. Set `return_soluti
on_if_failed_early=True` to return the solution object up to the point where failure occurred.
2024-08-21 17:14:50.207 - [NOTICE] logger.func(7): Finish experiment simulation, took 5.191 s
```

In []: