Supplementary Information

Exploring the Effects of Cell-to-Cell Variability on Battery Aging through Stochastic Simulation Techniques

[1] Elias Barbers[1,2,3,z], Friedrich Emanuel Hust[2], Felix Emil Arthur Hildenbrand[2,3], Fabian Frie[2,3], Katharina Lilith Quade[2,3], Stephan Bihn[2,3], Dirk Uwe Sauer[2,1,3] and Philipp Dechent[2,3,z]
[1]Helmholtz Institute Münster (HI MS), IEK-12, Forschungszentrum Jülich, Campus Boulevard 89, 52066 Aachen, Germany
[2]Institute for Power Electronics and Electrical Drives (ISEA), RWTH Aachen University, Aachen, Germany
[3]Jülich Aachen Research Alliance, JARA-Energy, 52425 Jülich, Germany
[z]Corresponding Authors: Elias Barbers e.barbers@fz-juelich.de, Philipp Dechent philipp.dechent@googlemail.com

Parameterization of the Electrical Model

The fits conducted in the time and frequencey domain for the electrical model used in this work are shown in Figure S1. The parameters of the resulting electrical model are shown in detail in the figures S2 - S5. A deciption of the equivalent circuit is given in the main text of the paper in Figure 2. In addition to the circuit components inside each cell, wiring resistances were inserted into the electrical model of the battery pack. These resistances were set to a constant value of 1 mOhm. A verification of the cell model against a profile of current pulses is available in Figure S6.

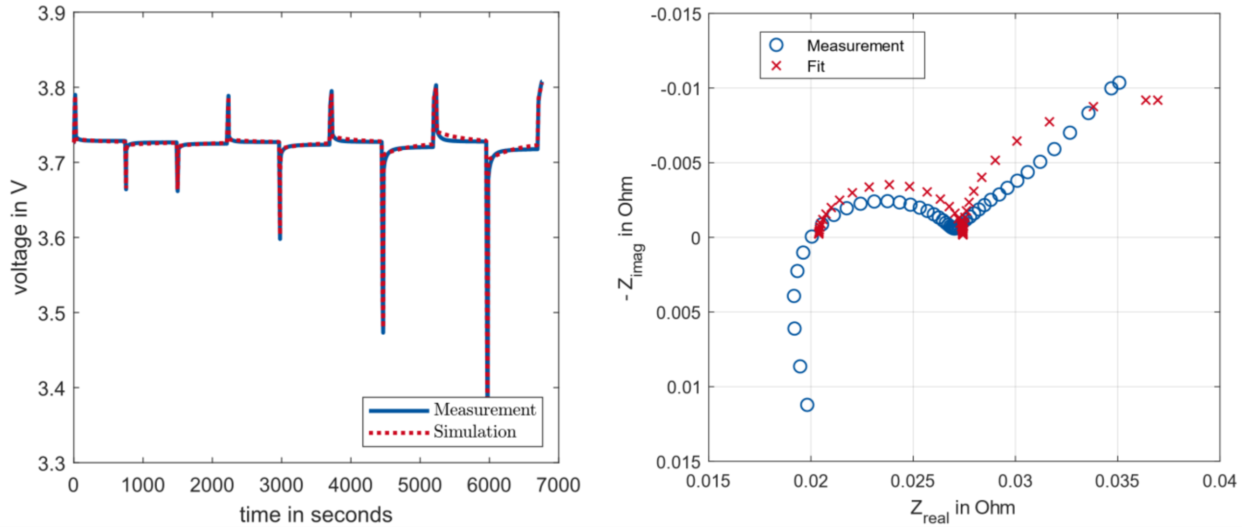

Figure S 1 Fit of the electrical model. a) Time domain b) Frequency domain

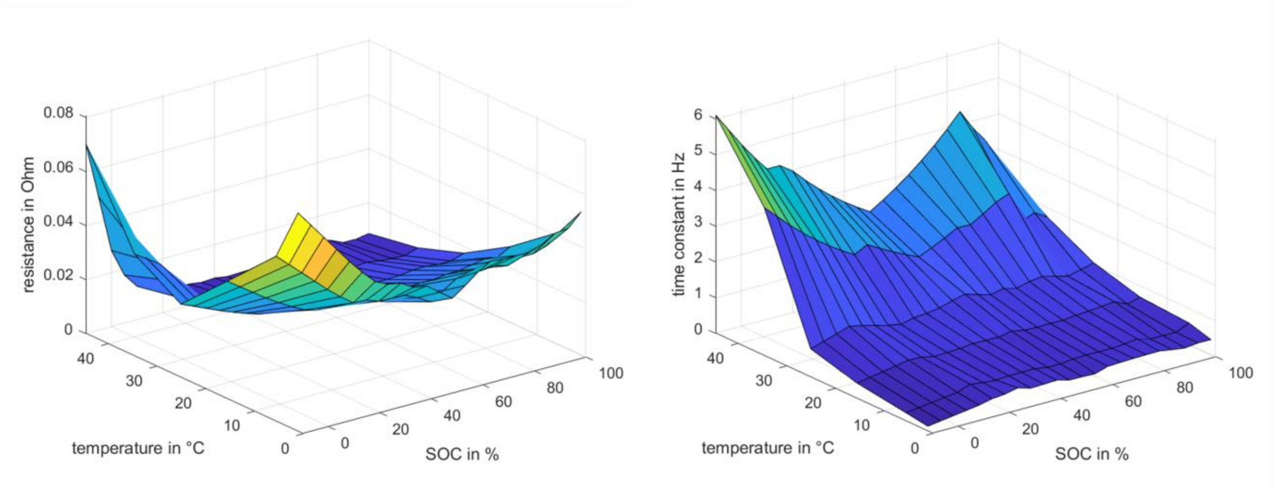

Figure S 2 Parameterization of the first RC element. a) Resistance b) Time constant

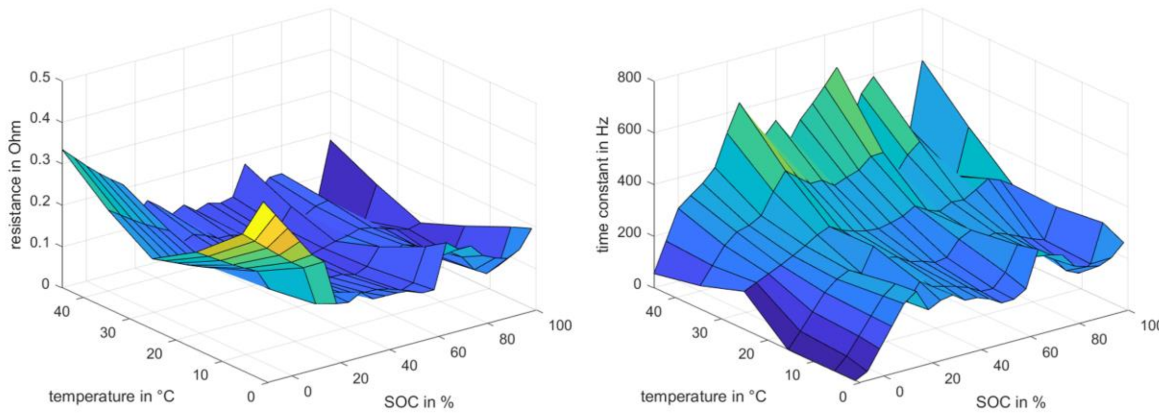

Figure S 3 Parameterization of the second RC element. a) Resistance b) Time constant

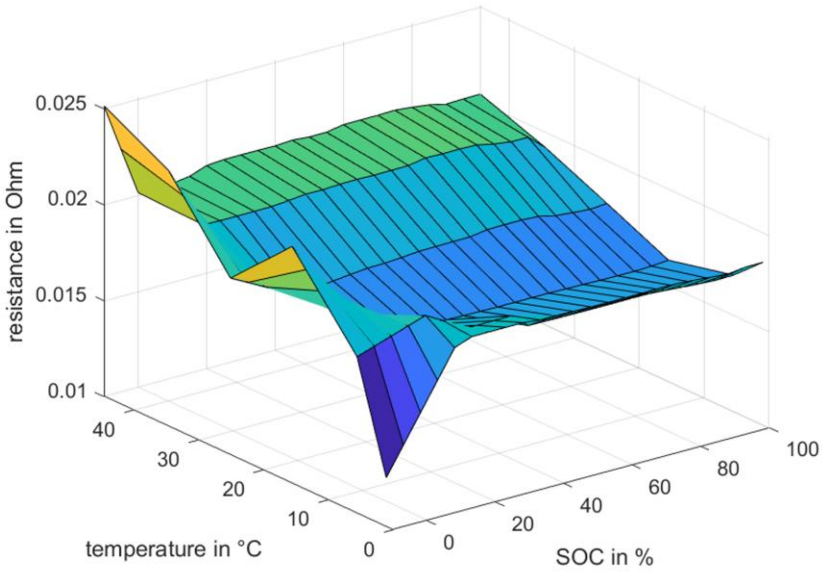

Figure S 4 Parameterization of the series resistance

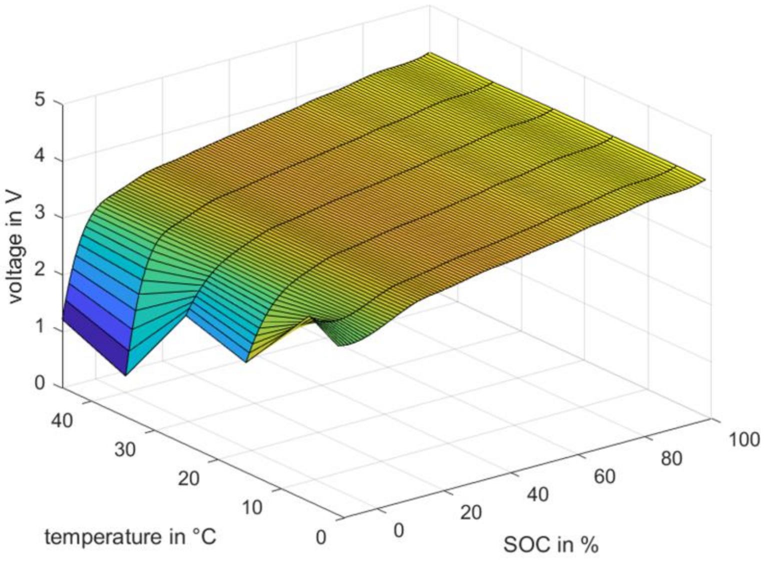

Figure S 5 Parameterization of the voltage source

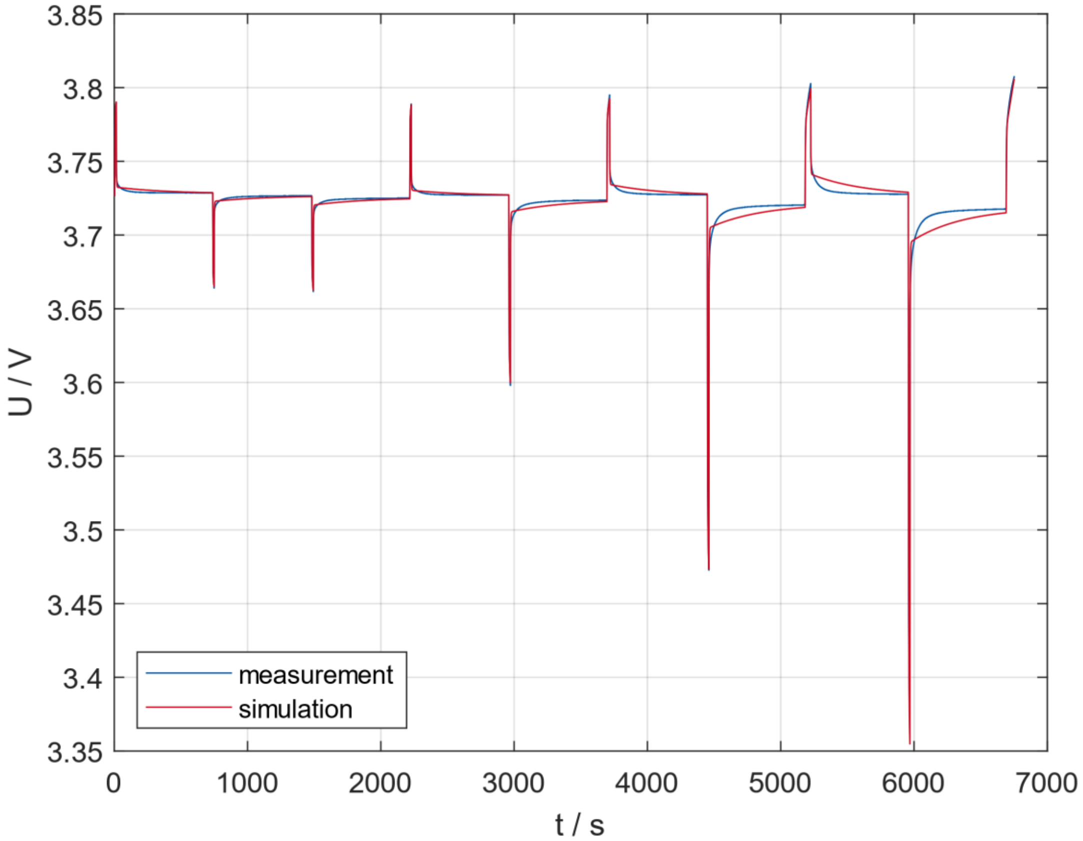

Figure S 6 Validation of the electrical model against pulses

Further explanation of the electrical simulation

A detailed description of the simulation framework is available in the PhD thesis of Hust [13]. To ensure the accessibility of the most relevant information, a description of the basic principles of the electrical and thermal simulation are reproduced below.

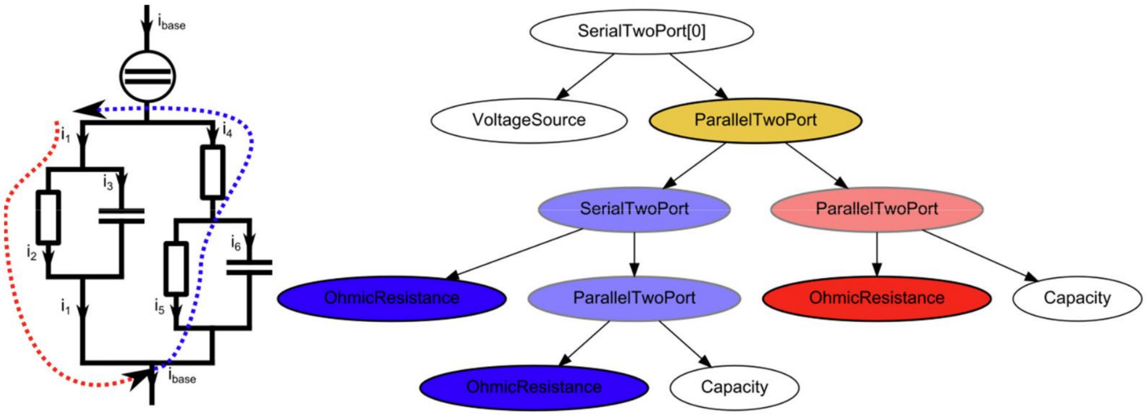

Figure S 7 Principle of the electrical model

In the figure above the derivation of one mesh equation can be seen. On the left-hand side an example circuit is presented. The red dotted curve depicts one branch of the parallel connection and the blue dotted curve represents the other branch. On the right-hand side, the tree representation of the network is shown. When trying to generate the mesh equation of the parallel connection (dark yellow bubble), the request is dispatched to all branches of the parallel connection. The dispatch calls a recursive function (GetVoltage) which gets the voltage equations for all sub-nodes. The GetVoltage call is delegated to the sub-nodes. Each sub-node decides how to handle the call. The elements will return the voltage equation. A serial connection will return the superposition of all equations of the sub-nodes. The parallel connection only returns the voltage equation of the first child as the other equations are equal. The GetVoltage function can be put into an algorithmic form in which three cases have to be considered: 1. In case the node is an element, the voltage equation for the element is returned. 2. For a serial connection a superposition of all sub-node's voltages is returned. 3. For a parallel connection the voltage equation of the first child is returned.

After deriving the voltages for each branch, a simple subtraction of the voltage from one branch with the other gives the result for one algebraic equation. All algebraic equations can be generated by iterating over all parallel connections in the tree.

These equations are combined with differential equations created by capacities and RC elements and form a Differential-Algebraic Equation system (DAE). This system is transformed into an ordinary differential equation system and solved in discrete time steps.

Further explanation of the thermal simulation

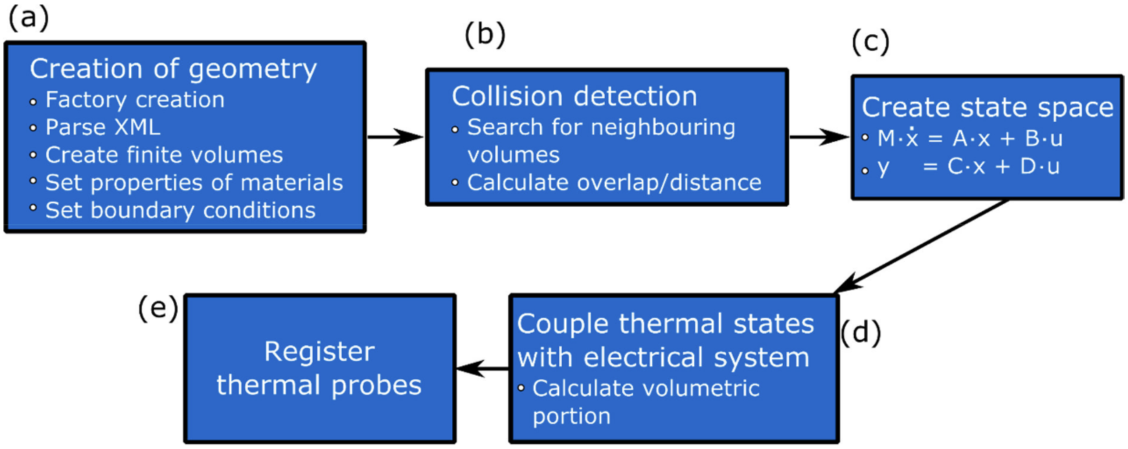

Figure S 8 Principle of the thermal model

In the figure above the abstract creation process of the thermal model can be seen. First of all, an XML-file is parsed in which all information for the thermal model is included. From this data the geometrical model is created (a). The creation process also includes the properties of the volumes such as density and thermal conductivity. Further, the boundary condition, also known as cooling, is set to the volumes. In the next step a collision algorithm (b) is checking whether any volumes are colliding or whether volumes are in close proximity (neighbor). For volumes with neighbors, the area overlap is calculated. Additionally, the distance from the volume's node to each surface is calculated. This enables a faster calculation of the heat conductivity between nodes. From the properties of the volume and its neighbors the state space equations (c) are derived with temperatures as one of the outputs. The state space equation can be similarly described as in the electrical model.

$$M \cdot \dot{x} = A_{G,Th} \cdot x - \left(A_{cooling}(x) \cdot x + c_{cooling}(x)\right) + c_{gen}$$

$A_{G,Th}$ represents the thermal conductivity between two volumes. The matrix is symmetrical with only negative values on the diagonal. All other values are positive or zero. The sum over a row or a column is equal to zero. $A_{cooling}(x) \cdot x + c_{cooling}(x)$ represents the linearization of the cooling at the temperature x. c_{gen} is the heat provided by the electrical model. Dirichlet boundaries are influencing $A_{cooling}$ whereas $c_{cooling}$ is influenced by the Neumann boundaries. All cooling processes are linearized in every simulation step. The temperatures are coupled to the electrical systems (d). As the discretization of the electrical and thermal system can differ, a volumetric coefficient needs to be determined for propagation. In the last step (e), thermal probes are set to specified volumes to get additional output.

Passive balancing current

The simulation of passive balancing currents is inherent in the setup of the simulation framework. With different states of charges, after for example a discharge due to capacity and internal resistance differences, the cells within a parallel connection will balance each other while relaxing, thus reducing the efficiency of the system Figure S 9 shows these balancing currents for cells during the first aging step (new cells) and the last aging step (aged cells) of Simulation 10 for a point in the current profile where the pack current is zero. The currents for the aged cells are larger, as there is a higher spread of resistance, capacity, and SOC between them.

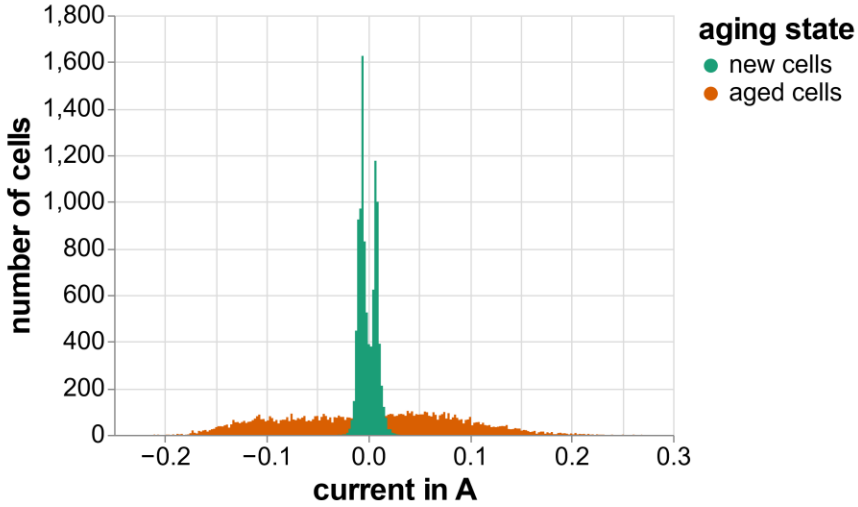

Figure S 9 Current for cells in a 20s5p topology (Simulation 10) when the pack current is zero.

Plots of individual distributions

Multiple figures within the paper show multiple distributions within one axis. To improve accessibility, and to enable a closer investigation of the plotted data, these figures are reproduced below with an individual axis for each distribution.

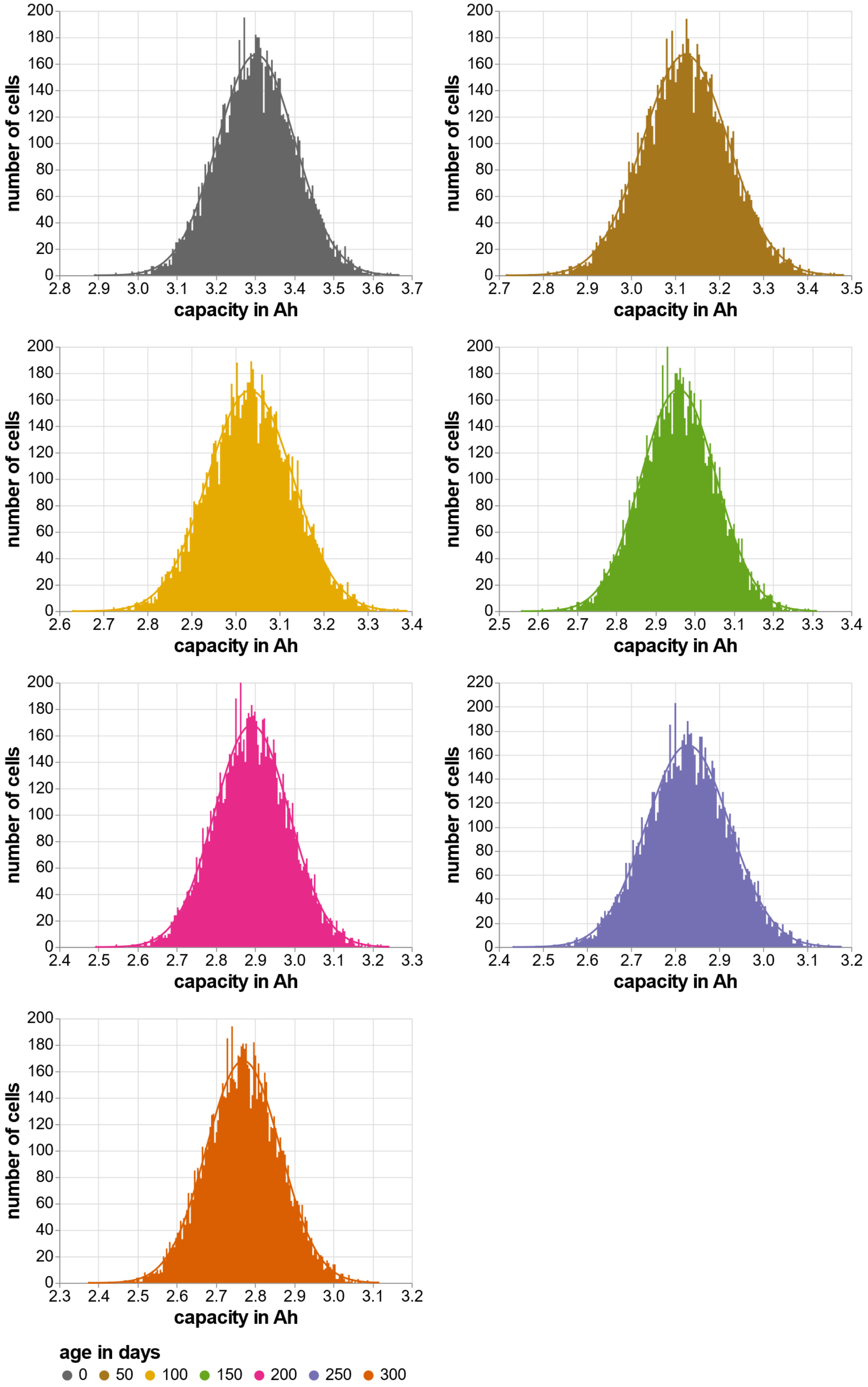

Figure S 10 Capacity distribution during Simulation 1 (see Fig. 5a)

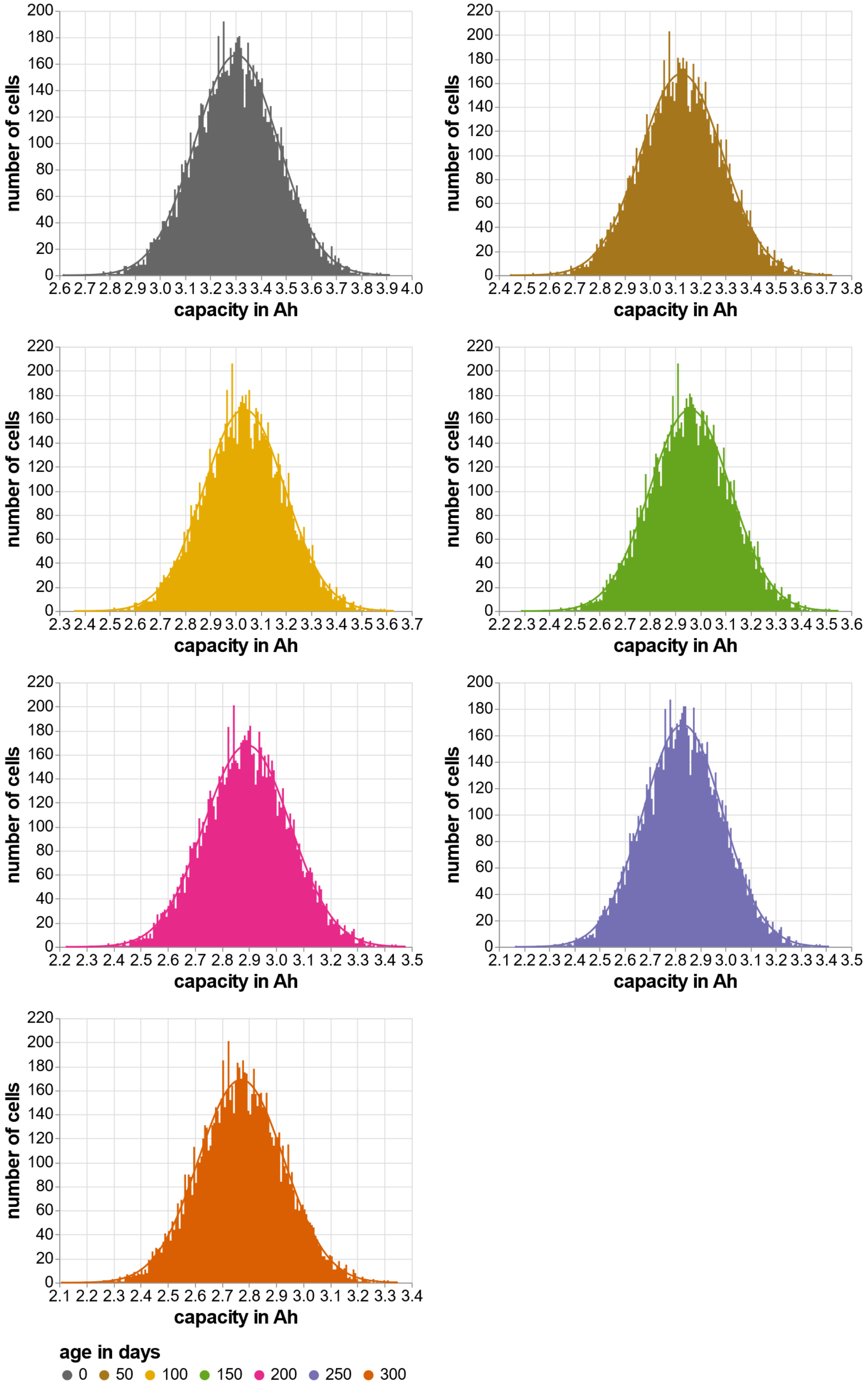

Figure S 11 Capacity distribution during Simulation 2 (see Fig. 5b)

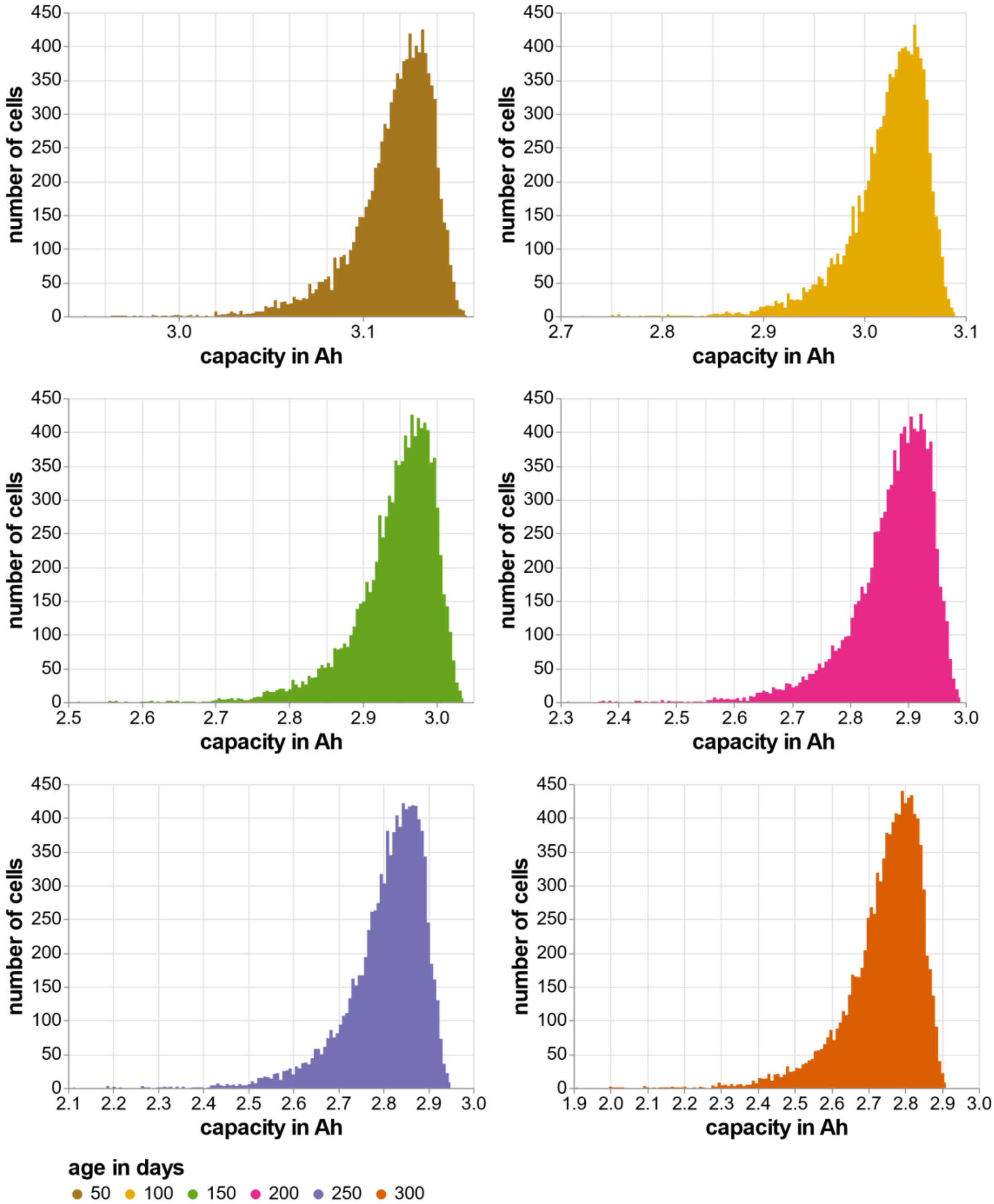

Figure S 12 Capacity distribution during Simulation 3 (see Fig. 6a)

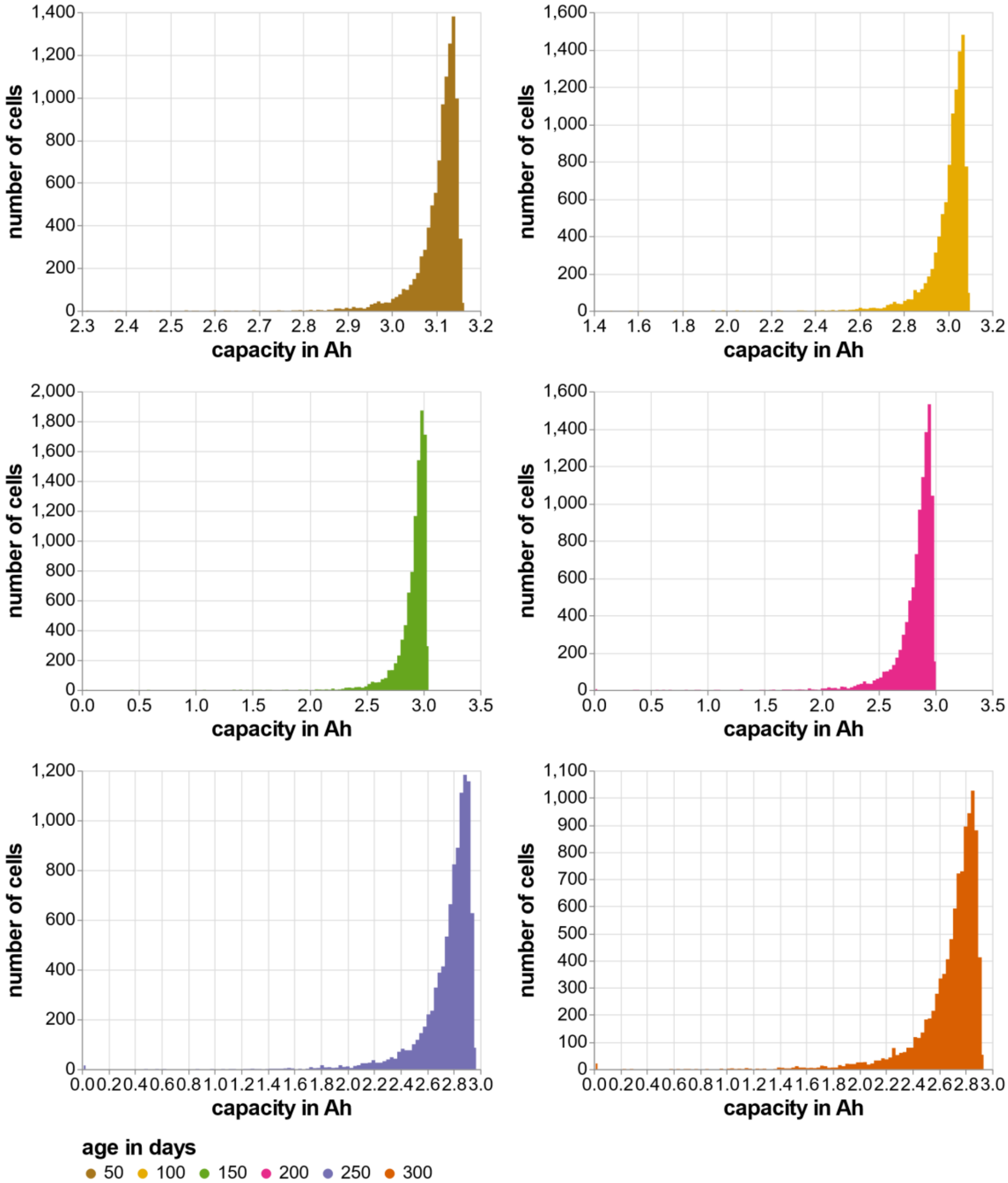

Figure S 13 Capacity distribution during Simulation 4 (see Fig. 6b)

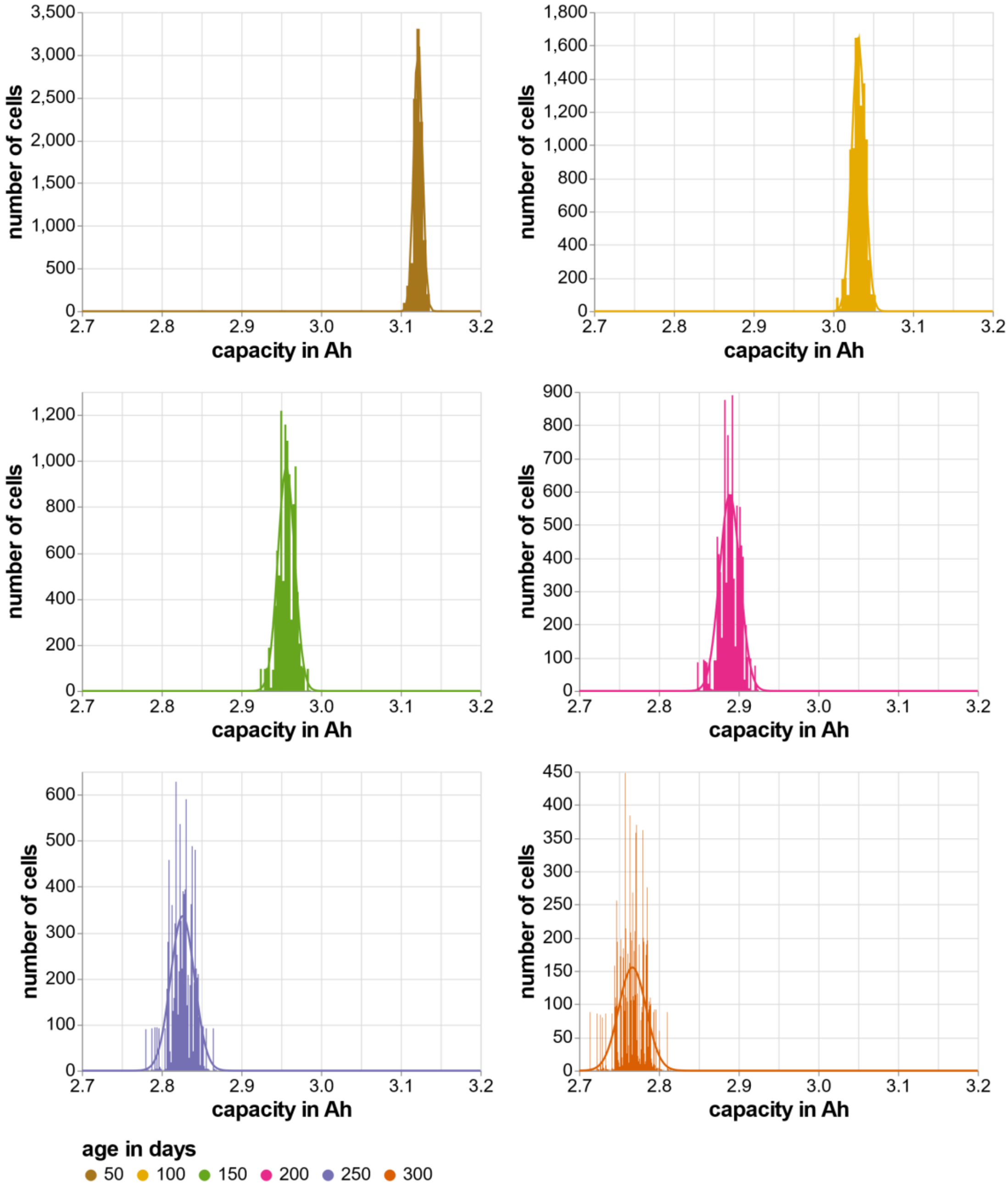

Figure S 14 Capacity distribution during Simulation 5 (see Fig. 7a)

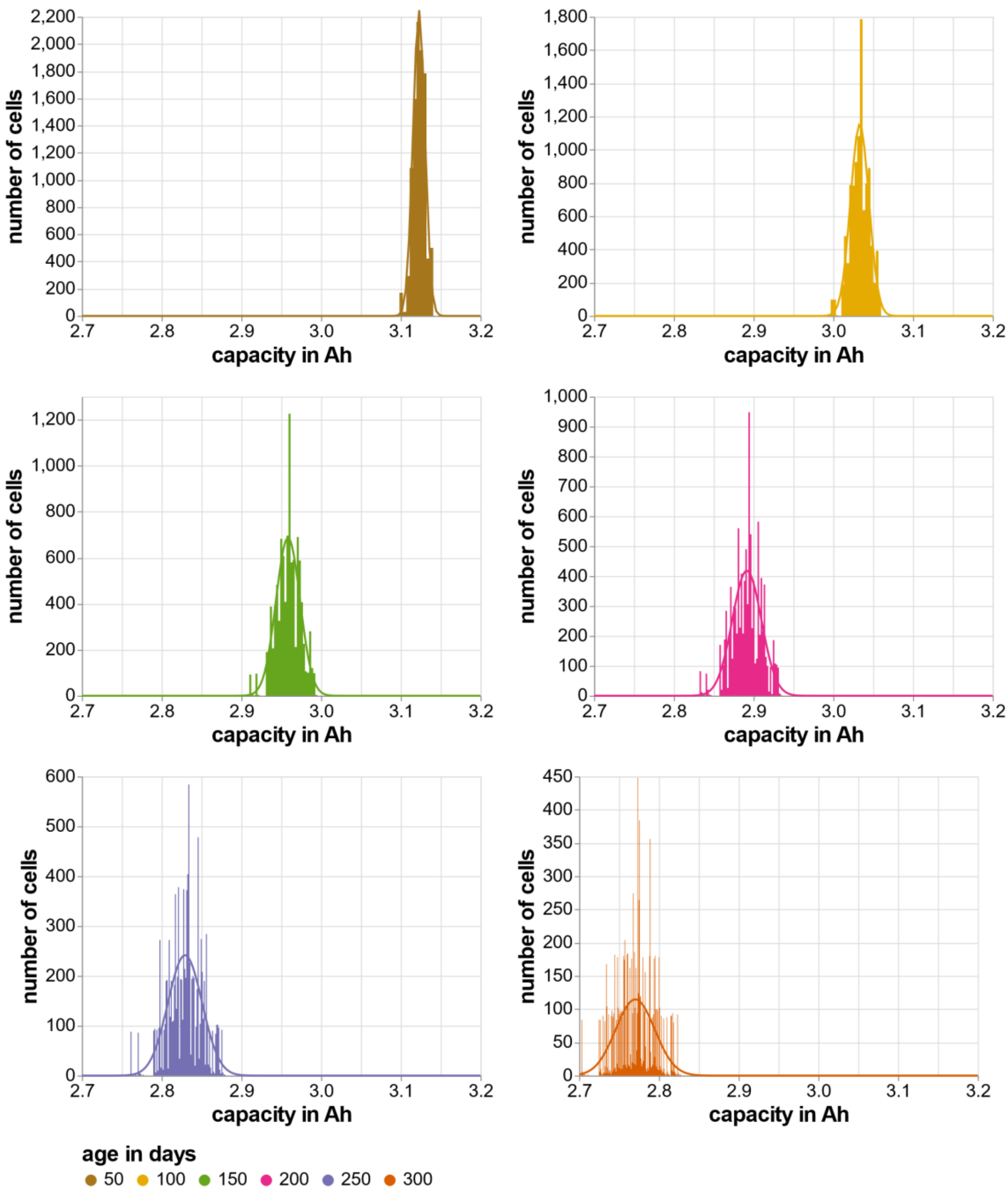

Figure S 15 Capacity distribution during Simulation 6 (see Fig. 7b)

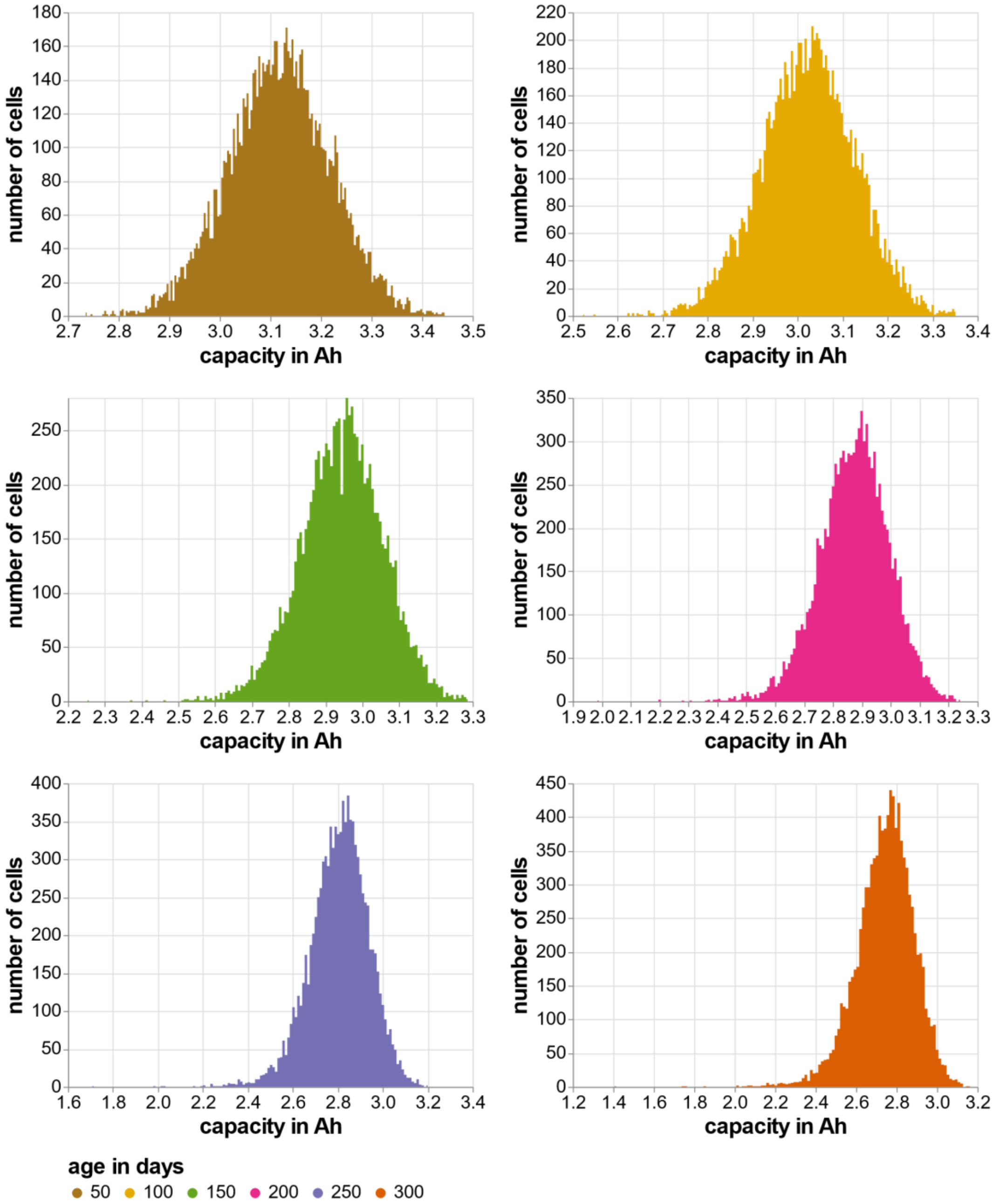

Figure S 16 Capacity distribution during Simulation 7 (see Fig. 8a)

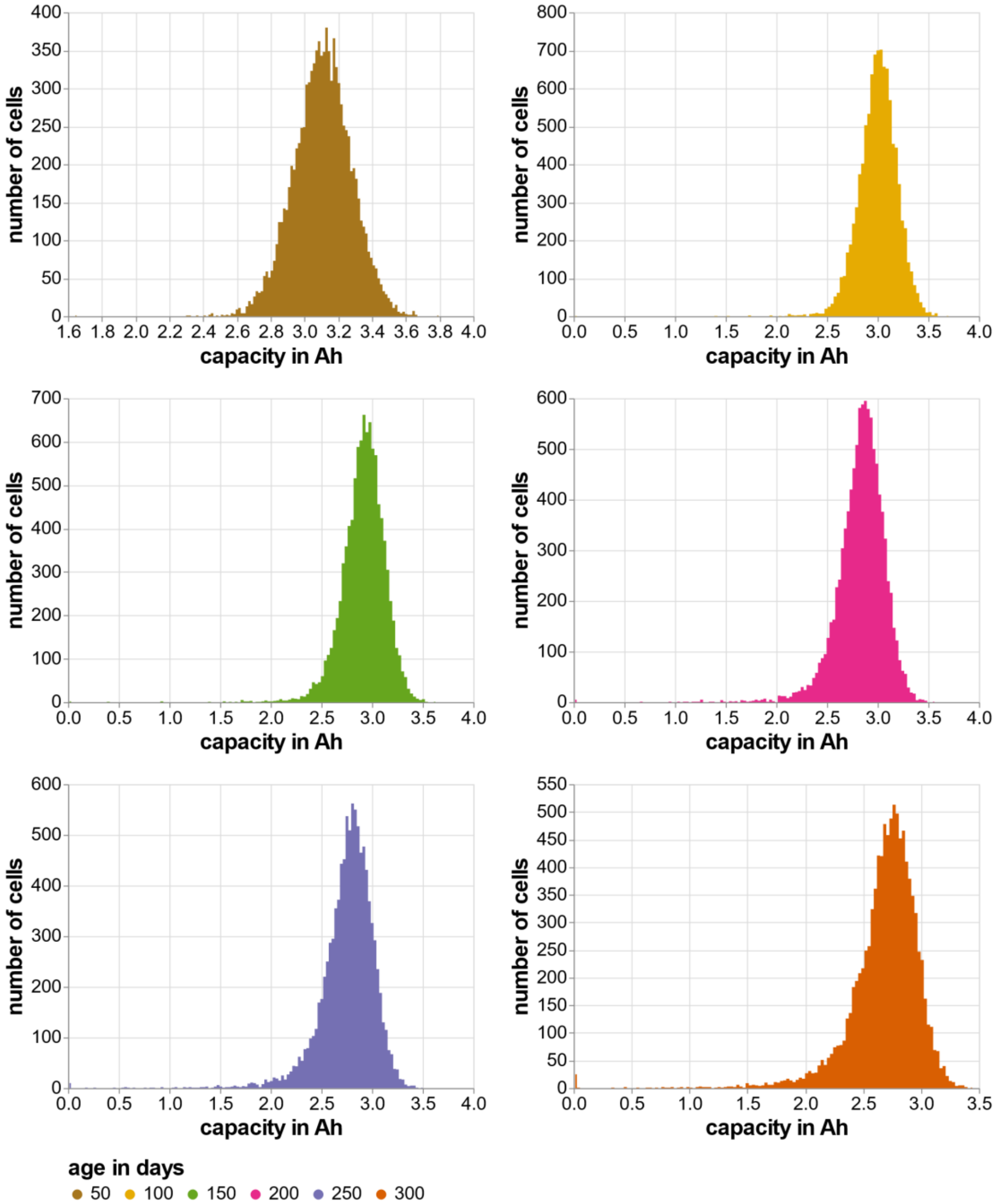

Figure S 17 Capacity distribution during Simulation 8 (see Fig. 8b)

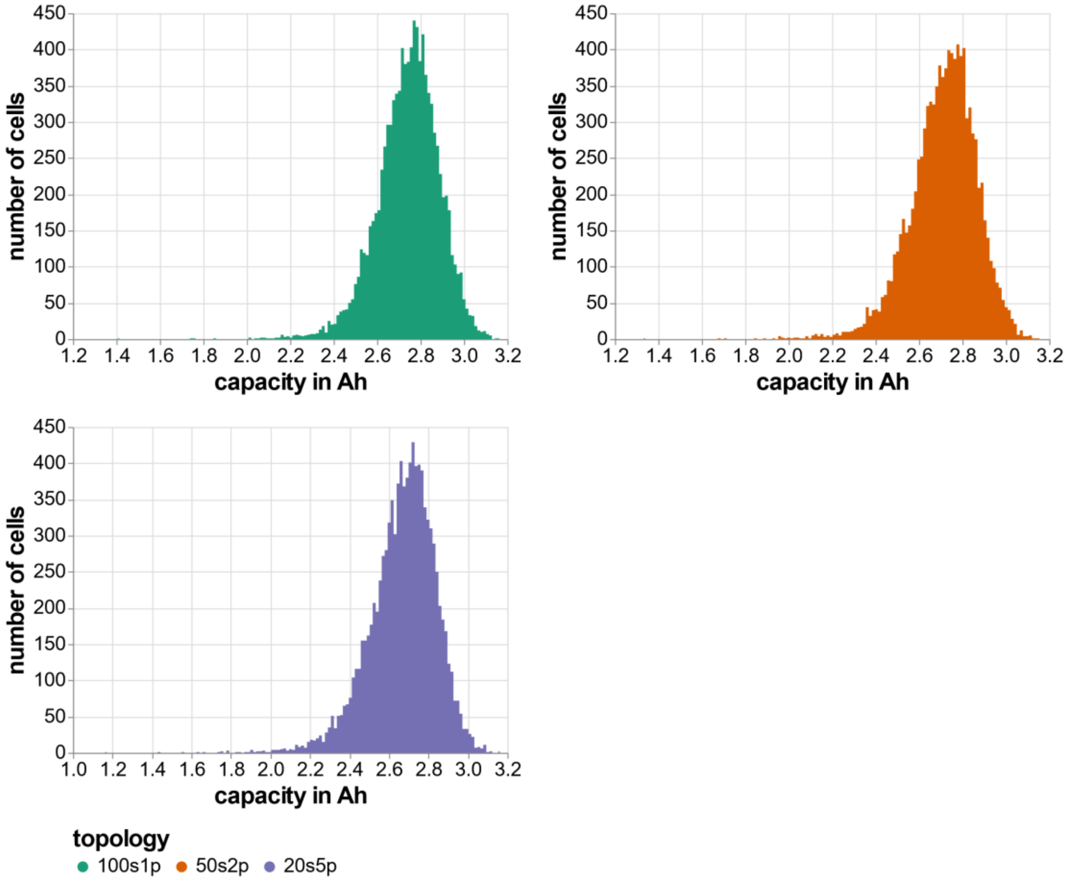

Figure S 18 Capacity distribution for different topologies (see Fig. 9)

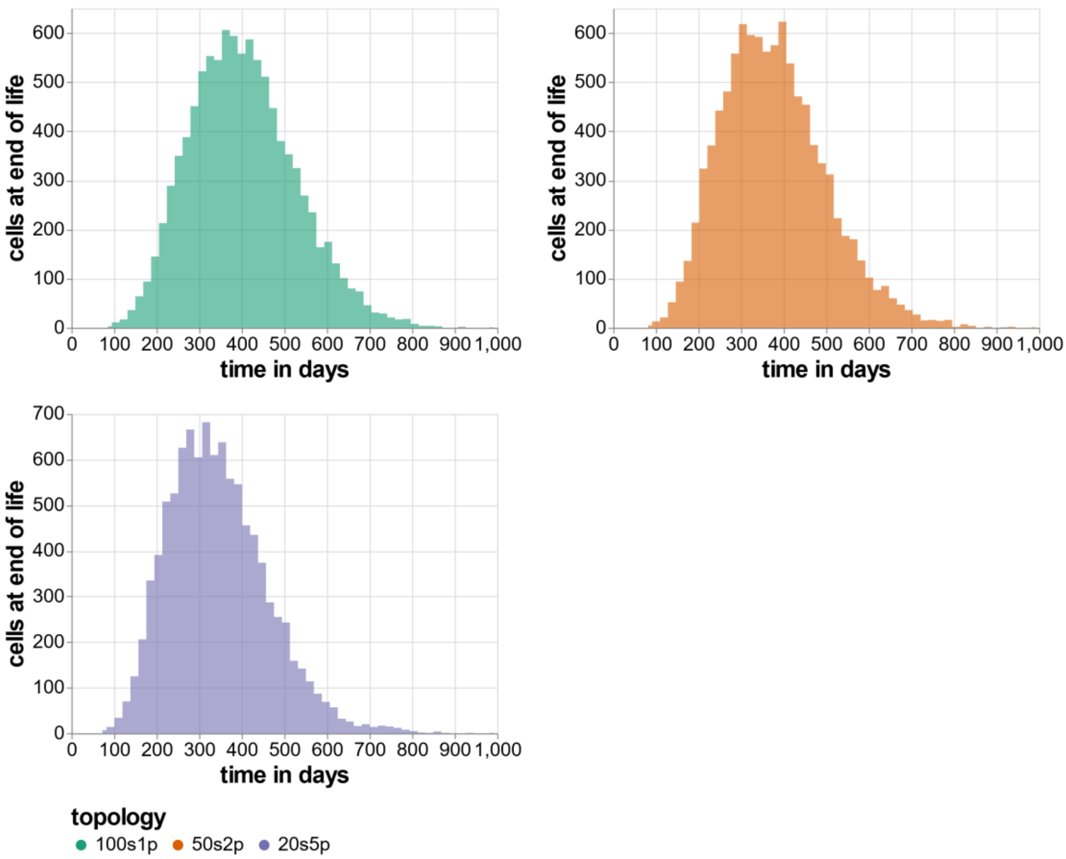

Figure S 19 Lifetime of cells for different topologies (see Fig. 11)

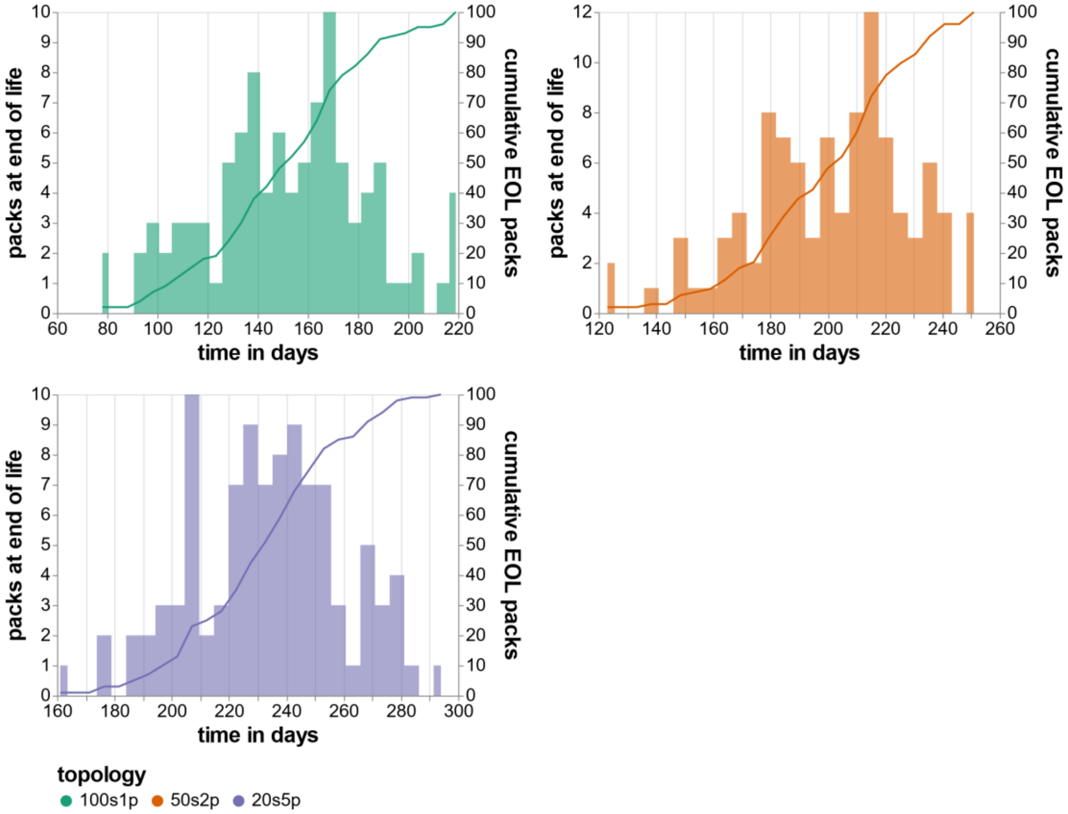

Figure S 20 Lifetime of packs for different topologies (see Fig. 12)