

Figure S1: Difference between measured and simulated temperature of the air pocket in the well base. The maximum difference between the predicted temperature and the measured temperature over the twelve time steps of the 3276s simulation was 0.6 °C at subzero temperatures. The error bars shown represent the uncertainty of the thermal probe at the well base, ± 0.3 °C.

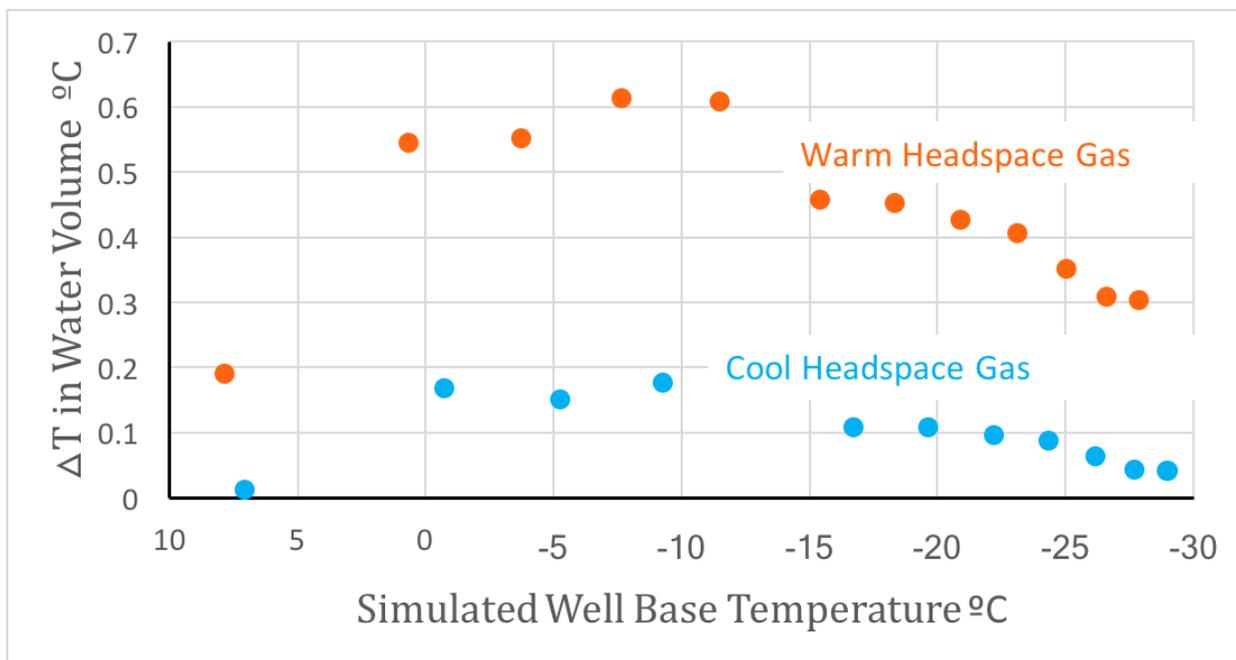


Figure S2: Simulated temperature stratification within the sample volume. The difference in simulated temperature between the top and bottom of the 50 μL sample volume is shown for the two simulations. Stratification of the sample volume under normal conditions as measured in the AIS reaches a maximum of 0.2 °C. Under the warmer headspace gas conditions as described in Sec. 3.2, stratification increases to a maximum of 0.6 °C.

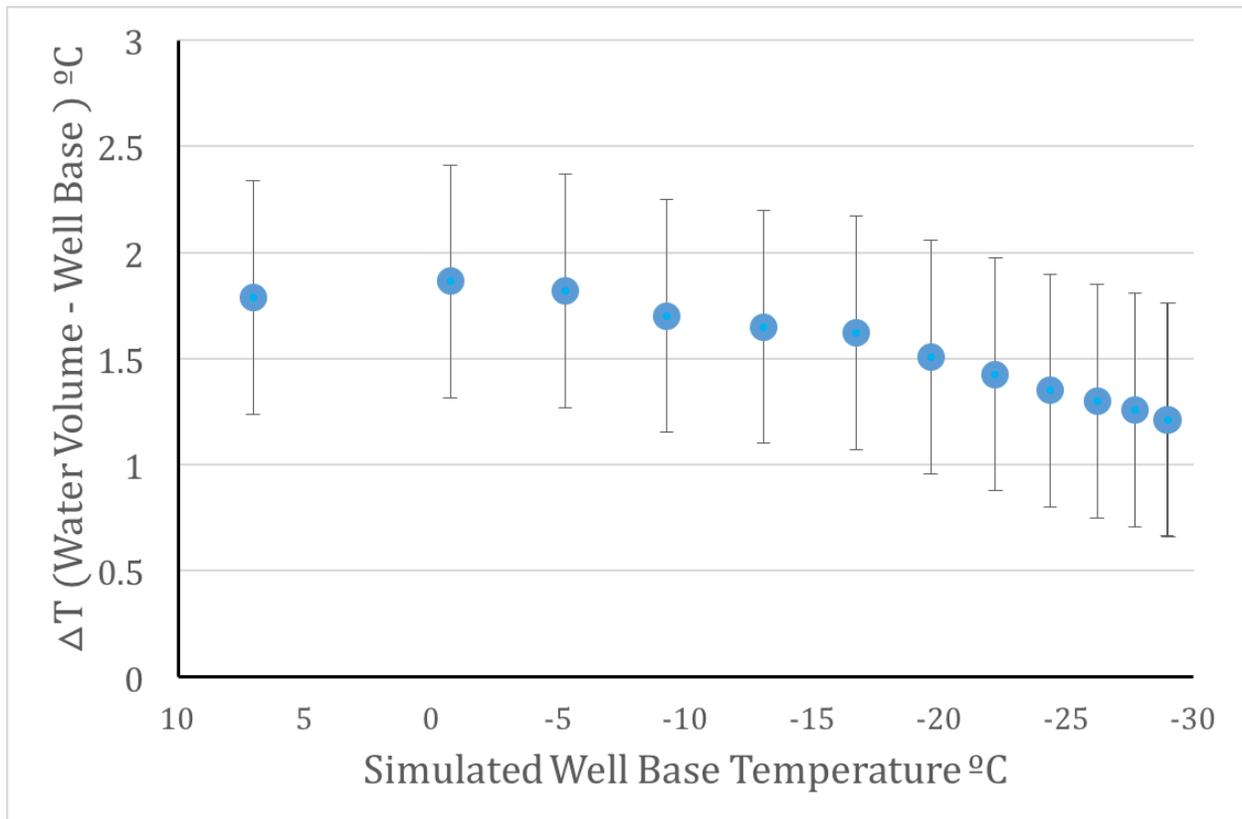


Figure S3: Simulated temperature offset between the sample volume and the well base. The average sample volume temperature is warmer than the air pocket in the well base throughout the 3276s simulation. Error bars reflect the uncertainty of the simulation based on the difference between measured and simulated temperature of the well base (see Fig. S1).

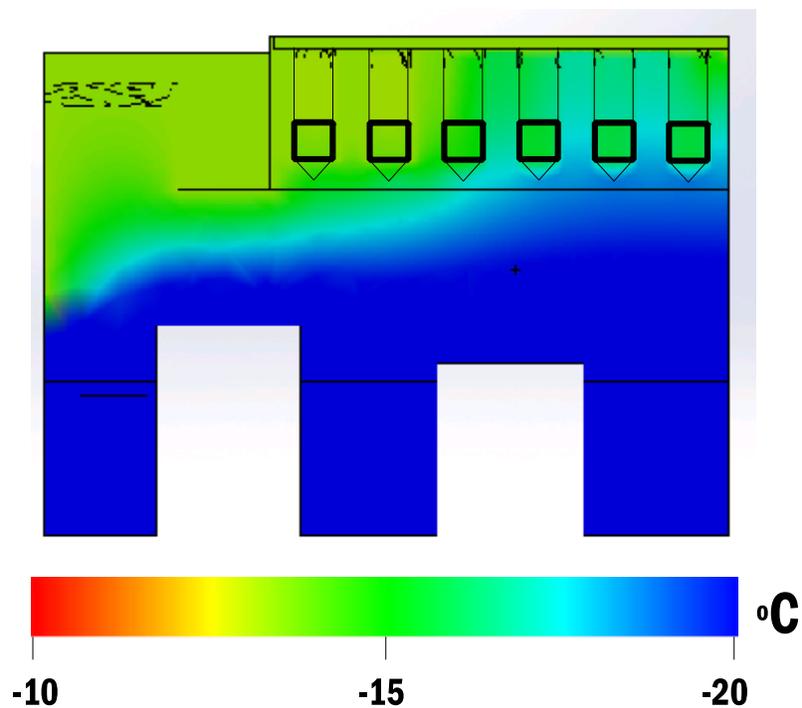


Figure S4: Spatial temperature gradient in sample volume temperature. Cross-section of top left quadrant of the well block (see Sec. 3.2 for details) at 1638 s. The sample volumes are outlined by the thick black rectangles. The leftmost sample volumes are closer to the outer edges of the well block, whereas the rightmost sample volumes are closer to the interior of the block. Thus, the leftmost sample volumes that are closer to the outer edges of the well block are warmer than the sample volumes along the interior of the well block, with a maximum difference of 2.2°C.