

Modeling the O₂ Purification in Large-Scale Cryostats

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This work develops a physics-based adsorption model to describe and predict oxygen removal in liquid argon cryostats. The model incorporates mass transport, pore diffusion, and adsorption mechanisms and was calibrated using experimental purification data through nonlinear parameter estimation. The validated model was then applied to large-scale cryogenic systems to predict purification performance and support scaling from laboratory experiments to detector-scale applications.

Mathematical Model

- Hypotheses:**
- isothermal system;
 - constant physical properties;
 - plug flow;
 - constant mass flow;
 - uniform bed porosity;
 - well-mixed tank.

System of partial differential equations (PDEs):

Fluid-phase

$$\frac{\partial C_i}{\partial t} = D_L \frac{\partial^2 C_i}{\partial z^2} - v_z \frac{\partial C_i}{\partial z} - \frac{(1 - \epsilon_b)}{\epsilon_b} K_{LaV} (C_i - Y_i)$$

Intra-particle fluid-phase

$$\frac{\partial Y_i}{\partial t} = \frac{K_{LaV}}{\epsilon_p} (C_i - Y_i) - \rho_s \frac{(1 - \epsilon_p)}{\epsilon_p} \frac{\partial q_i}{\partial t}$$

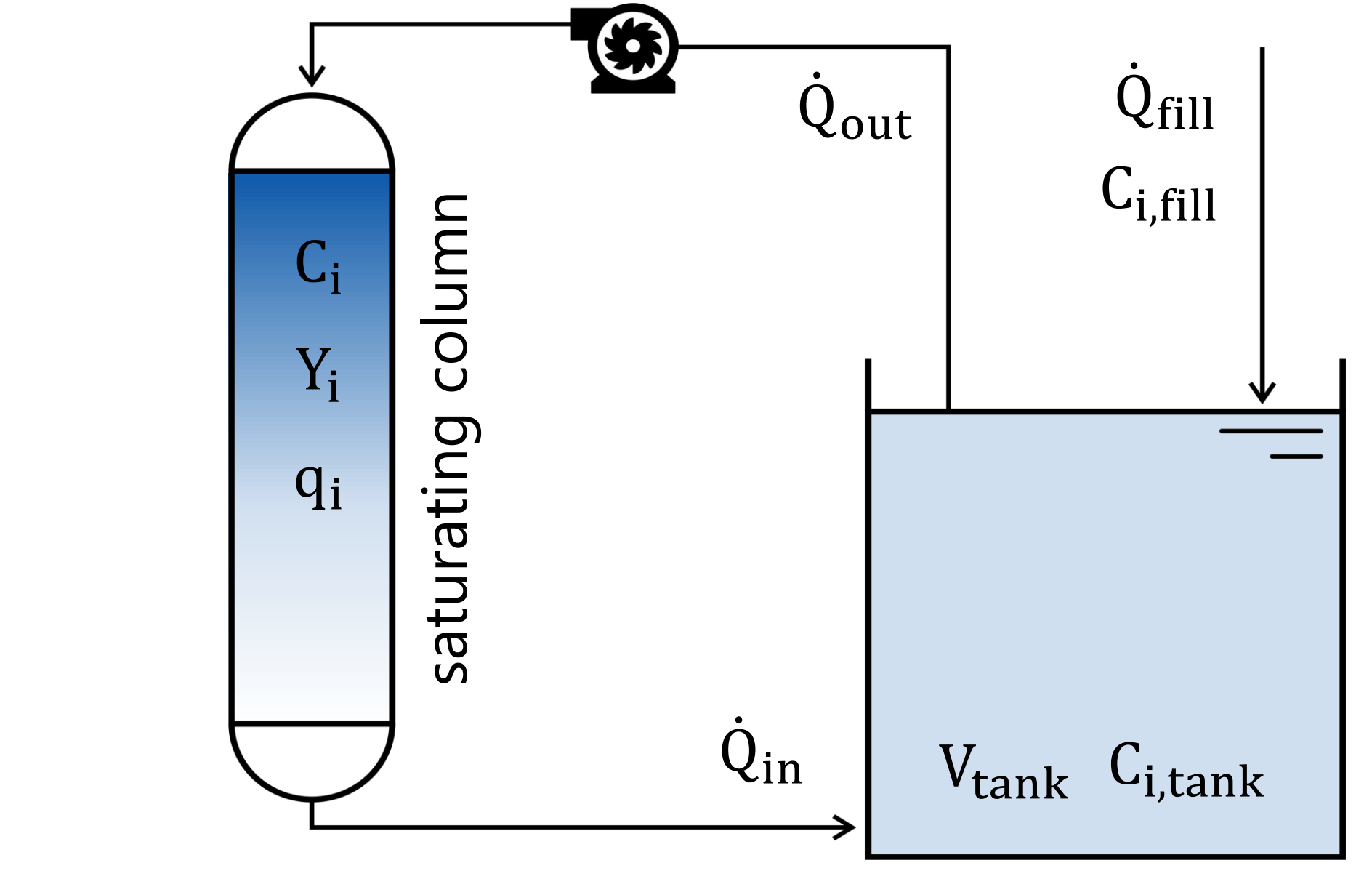
Storage Tank

$$\frac{dV_{\text{tank}}}{dt} = \dot{Q}_{\text{in}} - \dot{Q}_{\text{out}} + \dot{Q}_{\text{fill}}$$

$$\frac{dC_{i,\text{tank}}}{dt} = \frac{C_{i,\text{in}} \dot{Q}_{\text{in}}}{V_{\text{tank}}} - \frac{C_{i,\text{tank}} \dot{Q}_{\text{out}}}{V_{\text{tank}}} + \frac{C_{i,\text{fill}} \dot{Q}_{\text{fill}}}{V_{\text{tank}}} - \frac{C_{i,\text{in}}}{V_{\text{tank}}} \frac{dV_{\text{tank}}}{dt} + \frac{\dot{m}_{\text{leak}}}{V_{\text{tank}}}$$

Solid-phase

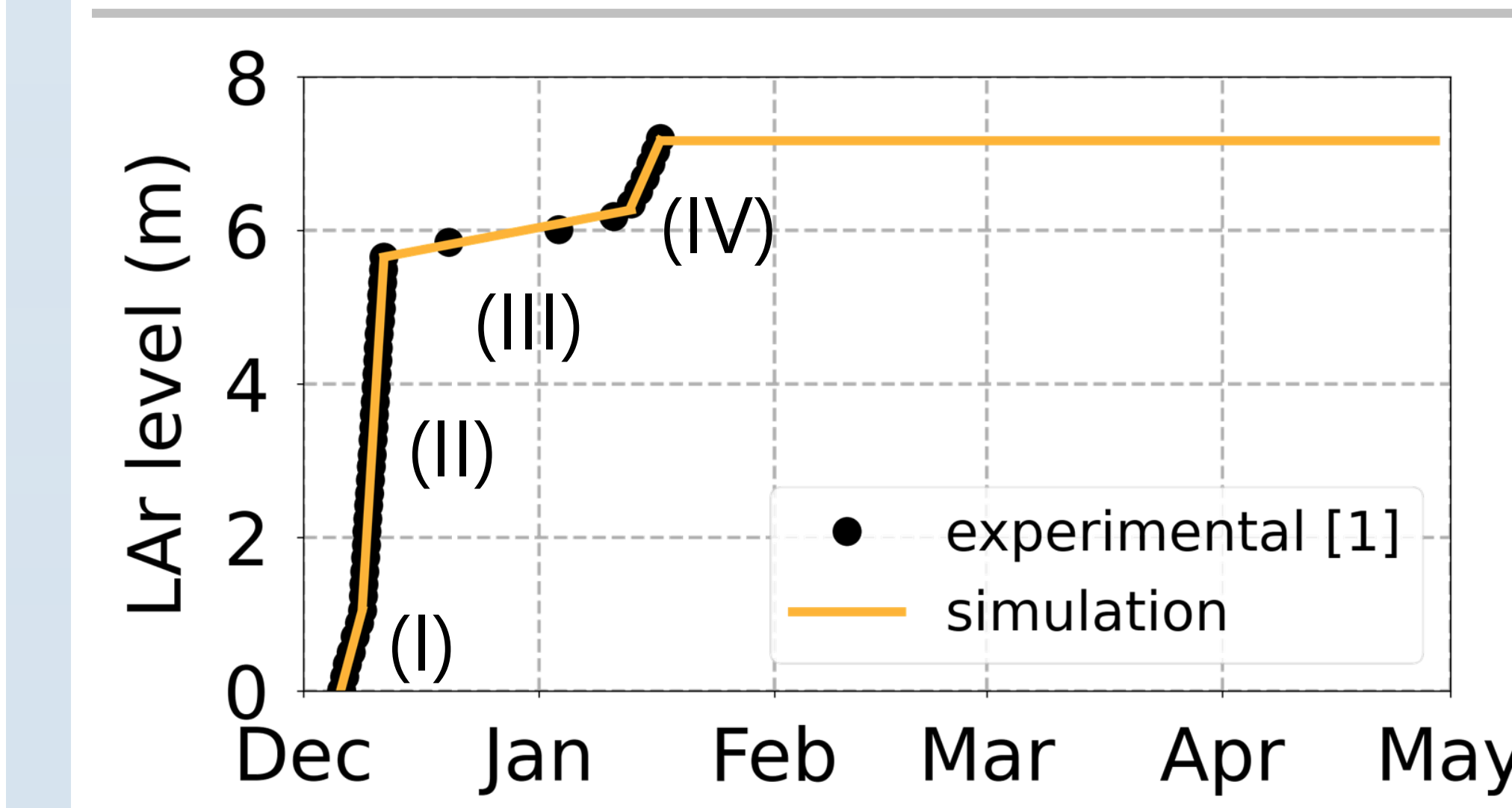
$$\frac{\partial q_i}{\partial t} = \frac{\partial f_{\text{eq}}(Y_i)}{\partial Y_i} \frac{\partial Y_i}{\partial t}$$



Langmuir Adsorption Isotherm:

$$f_{\text{eq}}(Y_i) = \frac{q_m k Y_i}{1 + k Y_i}$$

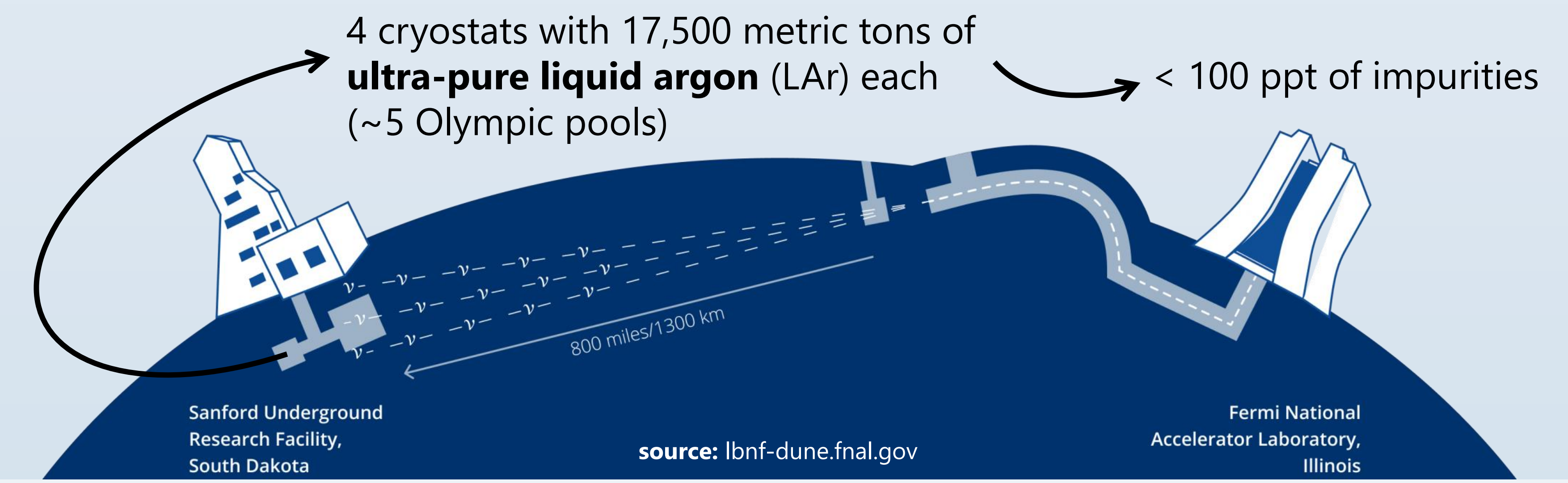
ProtoDUNE Cryostat Filling



- base area: 71.55 m²
- filling in 4 stages
- purification begins in stage (II)

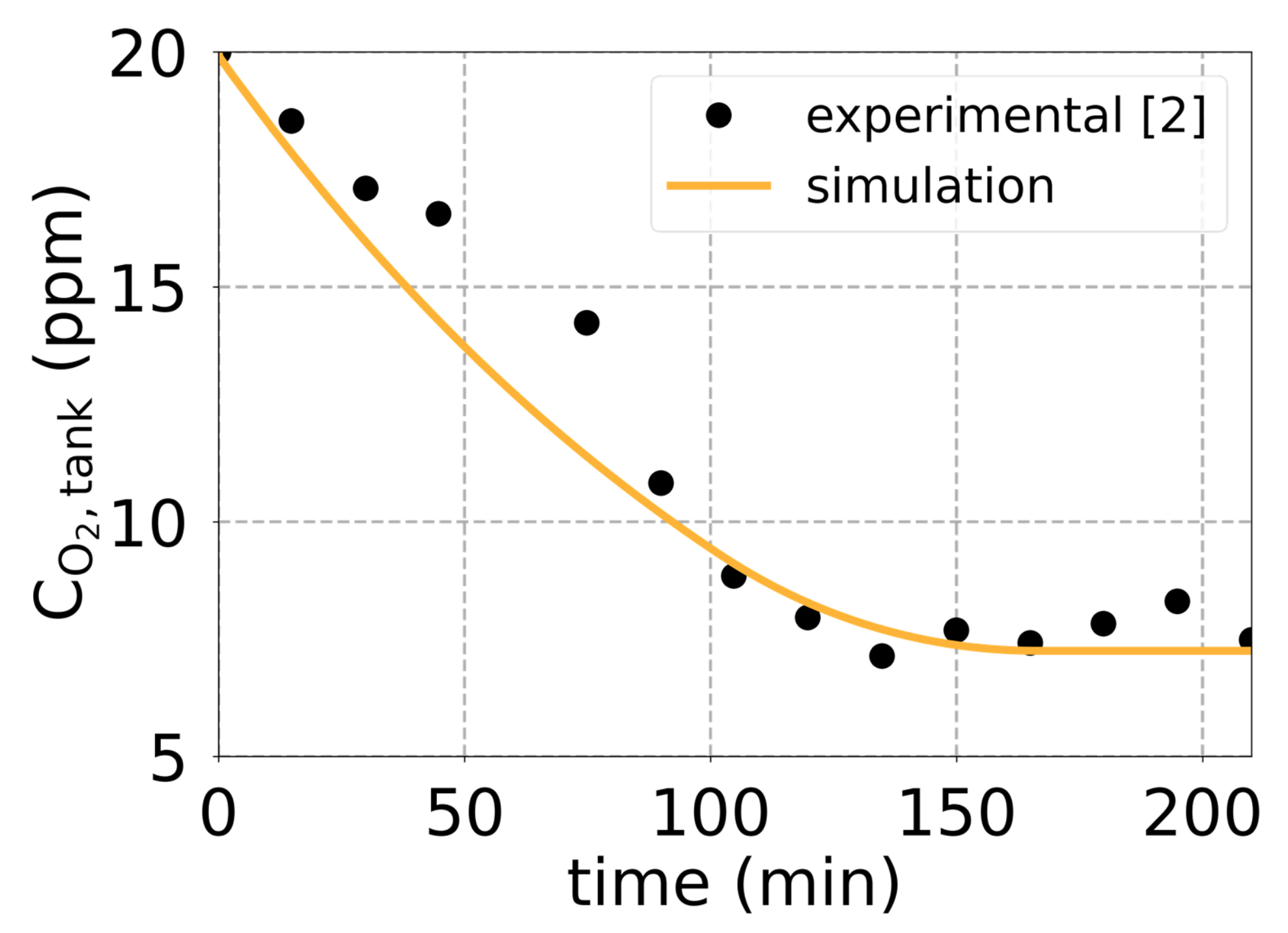
Deep Underground Neutrino Experiment

The **Long-Baseline Neutrino Facility (LBNF)**, located at the Sanford Underground Research Facility in Lead, South Dakota, hosts the **Deep Underground Neutrino Experiment (DUNE)**.



Adsorption Parameters

Purification Liquid Argon Cryostat (PuLArC) – 0.14 m³ of LAr:



2.44 kg BASF Cu Molecular Sieve
R² = 0.9573

Isotherm parameters	
q _m	1.66 × 10 ⁻³ kg/kg
k	1.74 × 10 ⁴ m ³ /kg

Predicting the ProtoDUNE



- 750 tons of Lar recirculating at 80.5 L/min
- 496.8 kg of BASF molecular sieve
- reaches 30 ppt after purification



References

- [1] Cavanna et al. *NP02 2025 Annual Report to the CERN-SPSC*. CERN-SPSC-2025-027 (2025).
- [2] A.M. Caffer et al., *Comparing the performance of CuO dispersive media for O₂ capturing in Liquid Argon*, JINST 20 (2025) C03043.

Acknowledgments

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