Computational Fluid Dynamics Surrogates for Carbon Capture Design Optimization

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Fundamental Problem

In this work, the physical phenomena under study are solvent-based post-combustion carbon capture systems (CCSs), in which CO₂ is captured through an absorption process caused by the interaction between a particular liquid solvent and the CO₂-laden gas inside a reactor column filled with packings. Figure 1 shows a representative section of the bench-scale column of a CCS, in which solvent is being injected into the column from the top ‘inlets’ and CO₂-laden gas (known as flue gas) is injected below.

Our data [1] was developed by our subject matter experts from PNNL, who implemented the CFD model of the CCS column in StarCCM+. 2D data was generated by taking a vertical slice of the 3D column and applying CFD to the CCS model.

1. Data Representation
   - Data is treated as an image (Fig. 2).
   - At each timestep, the CFD mesh is interpolated onto a regular grid and treated as an image frame.
   - Image processing techniques are fast and mature, but less accurate than mesh-based methods. Physics information is not easily preserved, and grid interpolation reduces accuracy.

2. Deeper Fluids (DF) Surrogates [2]
   - Latent-space creation: With DF, an autoencoder-based latent vector model (LVM) learns a physical field’s latent space & compressed data representation.
   - Latent-space simulation: The fast, latent integration network (LIN) learns to temporally advance the low-dimensional latent vectors.

3. Evaluation Metrics & Results
   - Error IA: relative error in the IA of the surrogate-simulated volume fraction field at the final timestep measures CCS efficiency prediction accuracy.
   - Error IA: relative error between IA and averaged over all test simulations’ timesteps; characteristics simplify between surrogate and CFD simulation.

Our primitive included a range of techniques for the physical phenomena under study: momentum equation, CFD models of counter-current solvent and gas flow, and fundamental problem of the CCS design. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL release number: LLNL-POST-846809. Contact: nguyen97@llnl.gov

Approach 1: Deeper Fluids Surrogates

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Approach 2: MeshGraphNets

Data Representation
- Data is treated as a graph (Fig. 5).
- Graph nodes/edges are derived from the CFD triangular mesh and store physics information at each mesh point as features.
- LIN’s mesh representation better preserves the physics by storing additional physical information as node data and avoiding interpolation.

2. MeshGraphNets (MGN) [3, 4]
- Encoding (E): Each node/edge computes an initial embedding from current timestep data.
- Message passing (M): Nodes/edges update embeddings by iteratively exchanging information with neighbors.
- Decoding (D): Final node embeddings are decoded as gradients (up) in physical space.
- Forward update (U): Physics data at each node is updated for the next time step.

Approach 3: End-to-End Surrogates

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2. End-to-End Surrogates
- With end-to-end surrogates, we are extending our work to train MGN on 3D meshes with millions of nodes, incorporating additional physics constraints, and optimize parameters to improve CO₂ capture efficiency.

Summary
- Our surrogates can quickly simulate CCS dynamics accurately for low-error IA predictions, circumventing the use of slower traditional CFD approaches.
- DF surrogates are fast, but must be retrained for new packing configurations and scales.
- MGN surrogates are transferable, providing a pathway to design optimization across different CCS design parameters (shape, size, resolution) and physics inputs (solvents, velocities).
- We are extending our work to train MGN on 3D meshes with millions of nodes, incorporate additional physics constraints, and optimize parameters to improve CO₂ capture efficiency.

References

Table 1. Quantitative evaluation of MGN approach
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Table 2. Quantitative evaluation of MGN approach

Figure 1. 3D CCS RC. Temporal evolution of the solvent distribution across the packed column

Figure 2. 2D volume fraction field

Figure 3. DF framework

Figure 4. Rel error of predicted IA and volume fraction at various latent dimensions

Figure 5. 2D Mesh of a vertical slice

Figure 6. MGN framework

Figure 7. Dataset packings and inlet velocities

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