Learning Conditionally Calibrated Equations of State for Direct Fired SCO2 Cycles with Deep Neural Networks

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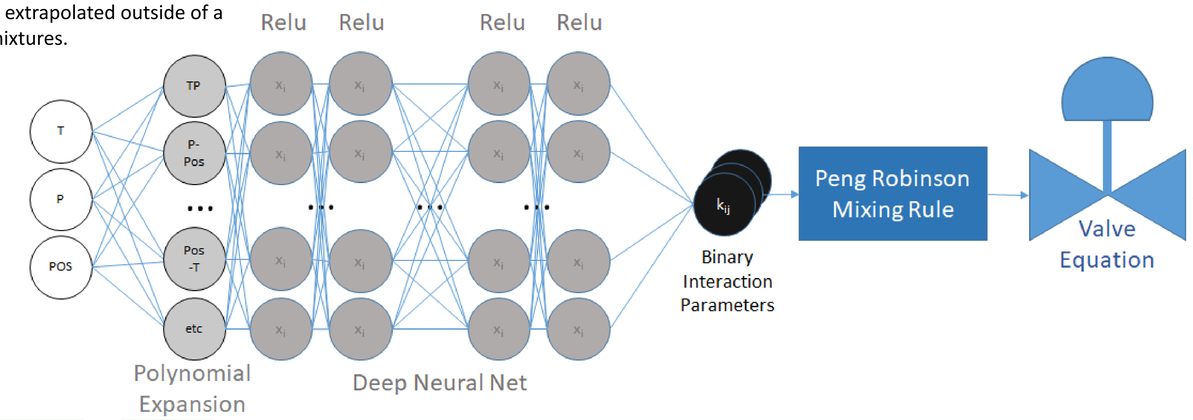
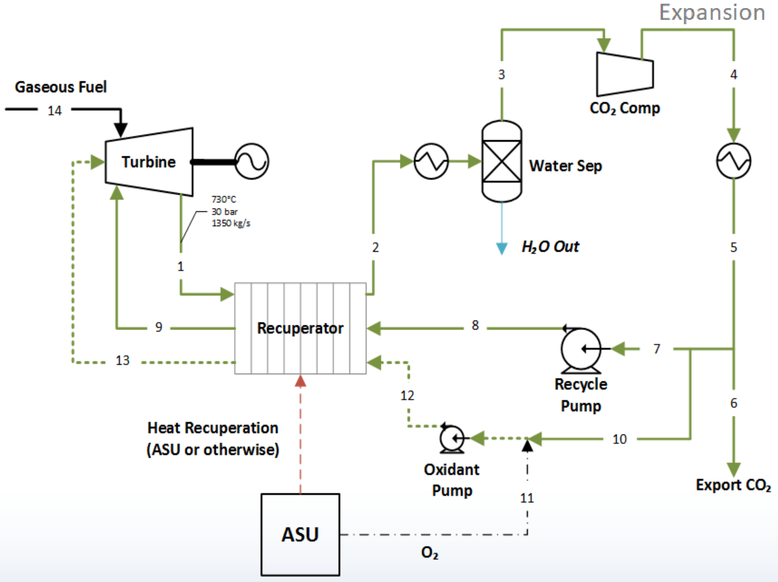
OVERVIEW

Equation of state (EOS) form the foundation for modeling the performance of carbon dioxide, and other, power cycles. Commercial software packages such as Aspen Plus rely on EOSs to inform and predict states of matter and interactions between matter under given conditions. Direct fired critical carbon dioxide systems offer unique challenges for standard equation of states found in the literature. In particular, the Allam Cycle utilizes a high-purity carbon dioxide working fluid across a wide range of conditions, including temperatures from 30C to 1150C and pressure from atmospheric pressure to 300 bar. As with all direct fired systems, it will have impurities in the working fluid that impact key engineering variables that are derived from the chosen equation of state. Peng-Robinson (PR) is a widely used EOS to describe the thermo-physical properties of pure CO2 and its mixtures in process modeling packages for power, oil, gas, and petrochemical industries applications. The most common methodology of calibrating the PR EOS in mixtures is by using binary interaction parameters (k_{ij}) which are typically experimentally derived in controlled volume systems and combined using the Van der Waals mixing rules. However, inaccuracies in predictions from most calibrations increase when extrapolated outside of a narrow range of conditions, or when considering multi-species mixtures.

EXPERIMENTAL SETUP

This paper presents a unique and broadly applicable methodology, treating these calibration parameters not as static, or sometimes temperature-dependent, quantities, estimated *in vitro,* but instead as *learned functions* allowed access to arbitrary side information, which is termed herein as *conditional calibration.* These functions are calibrated holistically, with respect to an entire system, rather than as independent scalar parameters learned through experiment, using the differentiability of the entire process model to enable gradient-based learning. In this work, it is demonstrated that a small but deep multi-layer neural network, generating the interaction parameters of a simple PR EOS-based model of a valve, significantly outperforms fixed parameter models in a pair of synthetic experiments.





EOS Ex.	Function Form	Year	Mixing Rule
PR	$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)}$	1976	$a = \sum_i \sum_j x_i x_j a_i^{\frac{1}{2}} a_j^{\frac{1}{2}} (1 -$

The first attempts to match a set of simulation data from a more sophisticated valve model using a simple model whose parameters are not fixed but generated, allowed access to temperature, pressure, and other features of the valve. The second adds an additional physically plausible pressure perturbation on top of the simulation. In both cases, the relative reductions in error are on the order of 40-50% to the simulated baseline by allowing the model to conditionally calibrate, while the fundamental physical grounding in cubic EOS models keeps the "black-box" learner reined in and easy to estimate, leveraging the best parts of machine learning and chemical process modeling. The aim is not only to offer a powerful methodology for empirically updating existing cubic equations of state with data from real plant environments, but also to advocate for a *flexible*, *conditional*, and *differentiable* approach to computational chemical engineering and process optimization in general.

RESULTS AND DISCUSSION

While the modeling technique imposes somewhat of an artificial constraint, it is meant to demonstrate several things:

1. Laboriously calculated binary EOS parameters can be calibrated on-the-fly to custom, non-idealized systems with heterogeneous conditions and multi-species mixtures in a way that is both less time consuming and more accurate within its area of data input.
2. Powerful conditional machine learning models like DNNs, allowing arbitrary covariates and side information to inform their predictions, can be safely "regularized", trained on little data, and prevented from overfitting by allowing them to only affect certain parameters of a semi-empirical model derived from reasonable physical principles, like cubic EOS, rather than having to learn a whole DNN-based EOS from scratch with the attendant burdens of massive training data and apprehensions regarding non-physicality.
3. Tunable semi-physical degrees of freedom in a process model, rather than posing estimation challenges in vitro, should be looked at as opportunities to fit directly in vivo to complex systems through automatic differentiation, with modern machine learning methods providing powerful tools to condition on sensors and other side information.

Model	Perturbed	Test AAD %
Standard k_{ij}	Yes	0.7052
Learned k_{ij} (fixed)		0.6625
Conditional Calibrated k_{ij}		
Depth		
2		0.5213
4		0.4112
6		0.3752
8		0.3703
Standard k_{ij}	No	0.4417
Learned k_{ij} (fixed)		0.4205
Conditional Calibrated k_{ij}		
Depth		
2		0.3659
4		0.3574
6		0.2334
8		0.2569