

Synthesis of Local Thermo-Physical Models Using Genetic Programming

Ying Zhang, and Aydin K. Sunol, Department of Chemical Engineering,
University of South Florida, Tampa FL 33620

Abstract:

Local thermodynamic models are practical alternatives to computationally expensive rigorous models that involve implicit computational procedures and often complement them to accelerate computation for run time optimization and control. Human-centered strategies for development of these models are based on approximation of theoretical models. Genetic Programming (GP) system can extract knowledge from the data in the form of symbolic expressions, i.e. a tree structure, which provides a means for function identification. It can be used to model and derive local thermodynamic models from the experimental data. This paper describes an adaptive hybrid system that is fully data driven automatic self-evolving to build appropriate approximating formulae for local model using genetic programming. No a priori information on the type of mixture (ideal/non ideal etc.) or assumption is necessary. At the end, the reliability of the model built by GP is tested using steady state and dynamic simulation.

The adaptive hybrid system, as shown in Figure 1, follows two tiers structure. The outer layer performs local thermodynamic model structure identification. The candidate model structure with unknown parameters will be passed to the inner layer. The inner layer then performs the parameter identification, which includes parameter structure identification (if the parameters display the dependency on certain variables) and parameter value estimation. In each layer, to optimize the terminal set and reduce the algorithm searching space, principal component analysis is performed before genetic programming based algorithm is applied.

Outer layer:

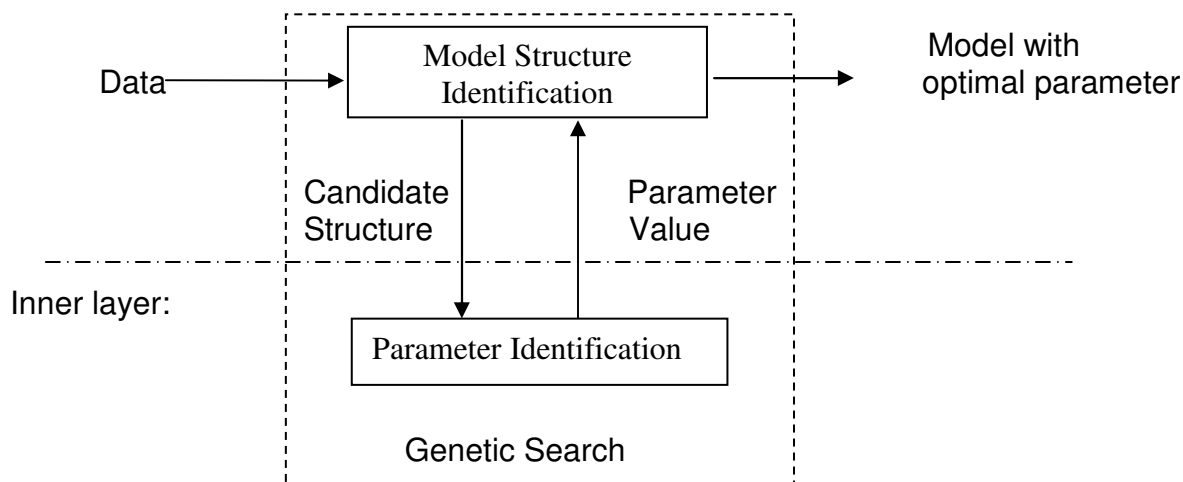


Figure 1 Hybrid System Structure for Structural and Parametric Optimization

The evolved K Models for Propylene-Propane near ideal solution and Acetone-Water strongly non-ideal solution have been studied. The results reveal that the hybrid system is able to find the explicit form of model that closely approximated the data in a relatively wide range while the accuracy is kept at an acceptable level. The composition-dependent local models developed have been shown to represent equilibrium ratios in a non-ideal vapor-liquid system with significantly greater accuracy than purely temperature-dependent local models that have been proposed in the past. The models have also been shown to accurately represent ideal mixture equilibrium ratios for a binary vapor-liquid system.