# New Technology for On-Demand Critically Evaluated Thermophysical Properties Data in Process Simulation

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The chemical process industries are faced with a myriad of challenges - from increased global competition, to the severe global economic down turn, and increased government regulations – just to name a few. In addressing these challenges, these industries are increasingly relying on process modeling tools to design, operate and optimize chemical processes. These tools include process simulation software (both steady state and dynamic), process synthesis, heat exchanger design programs, on-line deployment software, and on-line (or off-line) optimization software, among others. These programs enable engineers to predict the behavior of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. With reliable thermophysical property data, realistic operating conditions and the rigorous equipment models, they can simulate actual plant behavior. Thermophysical properties are keys to generating accurate simulation results that can be used with confidence. Inaccurate or incorrect thermophysical properties can lead to poor design or plants that do not operate as expected resulting in enormous economic loss and perhaps environmental harm. Therefore, process modeling software must strive to provide accurate, reliable and easily accessible thermophysical property calculation methods and data to enable efficient and robust process design. The problem is more challenging when dealing with new chemicals where no or little property information is known.

The traditional method of providing property data relies on a "static" database of pre-evaluated thermophysical property data. While this method "works" in principle, it cannot be used for compounds not already available in the database nor can it incorporates additional data that may become available until the next round of "static" evaluation exercise takes place. A better approach is to dynamically evaluate properties based on the current state of data and process requirements; that is, to develop property data "on-demand". Recently, researchers at the National Institute of Standards and Technology (NIST) have developed the concept of dynamic data evaluation and a program called ThermoData Engine (TDE) that implements this concept. The new concept of dynamic data evaluation relies on the availability of large-scale electronic databases that store essentially all experimental data known to date with detailed description of relevant metadata and uncertainties. The combination of these electronic databases with artificial intellectual expert-system software, designed to automatically generate recommended data based on the available experimental data and a system of prediction methods, leads to the ability to produce critically evaluated data dynamically. The dynamic data evaluation process dramatically reduces the effort and costs associated with developing the necessary thermophysical property data required by process simulation.

In this presentation, we will review past practice in obtaining the necessary thermophysical property data required in developing a process model. We will then describe a new workflow that utilizes the NIST dynamic data evaluation concept and ThermoData Engine that has been implemented into a process simulation software, Aspen Plus®. Illustrative examples will be given to demonstrate the benefits of the new methodology. Opportunities and future directions related to this new technology will also be discussed