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A Thermodynamic Library for Simulation and Optimization of Dynamic Processes ⋆

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Abstract: Process system tools, such as simulation and optimization of dynamic systems, are widely used in the process industries for development of operational strategies and control for process systems. These tools rely on thermodynamic models and many thermodynamic models have been developed for different compounds and mixtures. However, rigorous thermodynamic models are generally computationally intensive and not available as open-source libraries for process simulation and optimization. In this paper, we describe the application of a novel open-source rigorous thermodynamic library, ThermoLib, which is designed for dynamic simulation and optimization of vapor-liquid processes. ThermoLib is implemented in Matlab and C and uses cubic equations of state to compute vapor and liquid phase thermodynamic properties. The novelty of ThermoLib is that it provides analytical first and second order derivatives. These derivatives are needed for efficient dynamic simulation and optimization. The analytical derivatives improve the computational performance by a factor between 12 and 35 as compared to finite difference approximations. We present two examples that use ThermoLib routines in their implementations: (1) simulation of a vapor-compression cycle, and (2) optimal control of an isoenergetic-isochoric flash separation process. The ThermoLib software used in this paper is distributed as open-source software at www.psetools.org.

Keywords: Thermodynamic library, Process simulation, Dynamic optimization, Vapor compression cycle, Vapor-liquid equilibrium, Flash separation

1. INTRODUCTION

Rigorous thermodynamic computations of vapor and liquid properties (volume, enthalpy, entropy) constitute a significant part of the computations in the dynamic simulation and optimization of many industrial processes governed by vapor-liquid equilibrium. Such processes are ubiquitous and include power cycles, vapor compression cycles, refrigeration systems, vapor-liquid separations in tanks, distillation columns, and oil reservoirs modeled by compositional and thermal models. Thermodynamic models, such as equations of state (EOS) and activity coefficient models, are widely used in the process industries and represent a certain level of complexity. As process simulation and optimization software depends critically on thermodynamic property computations, it is crucial to the computational performance that such thermodynamic models are implemented efficiently. Simulation and gradient-based optimization of dynamic process systems governed by vapor-liquid equilibrium require in addition to the thermodynamic properties themselves also first and in many cases second order derivatives of the thermodynamic properties.

In this paper, we present a performance study of a recently developed open-source thermodynamic library, ThermoLib, which is designed for efficient dynamic simulation and optimization. It is implemented in Matlab and C. The novelty of ThermoLib is that it provides routines for evaluating analytical first and second order derivatives with respect to temperature, pressure, and mole numbers. The derivatives are obtained with symbolic differentiation. The library is based on parameters and correlations from the DIPPR database (Thomson, 1996), the Peng-Robinson (PR) EOS (Peng and Robinson, 1976), the Soave-Redlich-Kwong (SRK) EOS (Soave, 1972), and the van der Waals mixing rules (Shibata and Sandler, 1989). ThermoLib is an open-source library and is available from www.psetools.org (Ritschel et al., 2016). There are already a few open-source libraries such as the simulink toolbox T-MATS by Chapman et al. (2014) and a Matlab library by Martín et al. (2011). Furthermore, the CALPHAD software OpenCalphad developed by Sundman et al. (2015) contains an open-source module for evaluation of thermodynamic properties. However, none of these libraries provide both first and second order derivatives.

We present two examples that use ThermoLib routines in their implementations, namely simulation of a heat pump and dynamic optimization of an isoenergetic-isochoric flash separation process. Heat pumps are promising for the recovery of waste and ground heat and have numerous complex applications in heating and cooling, i.e. air

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conditioning, floor heating, cryogenic air distillation, drying processes, etc. The European Heat Pump Association (2015) has reported that a total heat pump capacity of approximately 6.6 GW was installed in Europe during 2014, producing 13 TWh of energy and reducing CO_2-equivalent emissions by 2.09 Mt. Consequently, efficient simulation of heat pump devices is important to the design of economically attractive control methodologies, and will contribute to energy savings in both household and industrial applications. In the second example, we consider separation of hydrogen sulfide (H_2S) from a gas condensate. This is an example of a multi-component vapor-liquid equilibrium process that appears in e.g. distillation columns and is ubiquitous in the oil and chemical process industries.

This paper is structured as follows. Section 2 gives a brief description of the ThermoLib interface and presents a set of performance tests of selected library routines. Section 3 presents simulations of the heat pump and Section 4 presents an optimal control strategy for the flash separation process. Conclusions are given in Section 5.

2. THERMODYNAMIC LIBRARY

This section briefly discusses the interfaces of the ThermoLib Matlab routines that are used in the heat pump simulations presented in Section 3 and the optimal flash separation presented in Section 4. Furthermore, we present a set of performance tests that illustrate the efficiency of selected library routines. ThermoLib is open-source software available at www.psetools.org and its methods are described by Ritschel et al. (2016).

2.1 ThermoLib Matlab Interface

Fig 1(a) shows a Matlab script that computes molar vapor and liquid enthalpy, entropy, and volume of Freon-12 which is one of the refrigerants that are used in the heat pump simulations. The thermodynamic properties are evaluated at a temperature of $T = 300$ K and a pressure of $P = 1$ MPa. The Thermolib routine LoadParams must be called before using any other routine. It loads DIPPR parameters and in this case also PR EOS parameters. The two routines PureRealVapHSV and PureRealLiqHSV return the thermodynamic properties together with first and second order temperature and pressure derivatives. Fig. 1(b) shows a Matlab script that computes enthalpy, entropy and volume of a hydrocarbon mixture. ThermoLib requires that the user specifies a set of binary interaction parameters, k_{ij}. These are all zero for hydrocarbons. The properties are evaluated at a temperature of $T = 300$ K and a pressure of $P = 10$ MPa. The two routines MixRealVapHSV and MixRealLiqHSV return the thermodynamic properties, vectors of first order derivatives, and matrices of second order derivatives.

2.2 Computational Performance of ThermoLib

Fig. 2 shows a set of performance tests that evaluate eight of the main routines in ThermoLib. The routines compute vapor and liquid properties of real and ideal mixtures as well as of pure components. Fig. 2(a) compares the efficiency of the library routines to numerical differentiation. The mixture routines are between 12 and 35 times faster than numerical differentiation, while the pure component routines are around 5 times faster. The speedup is lower for the pure component routines because they only evaluate temperature and pressure derivatives. Fig. 2(b) shows the computation time of the Matlab, C and Mex routines. The C routines are more than a hundred times faster than the Matlab routines and around ten times faster than the Mex routines. The order of magnitude ranges from milliseconds for the Matlab routines to microseconds for the C routines. Fig. 2(c) and 2(d) show the increase in computation time for the Matlab and C routines with respect to the number of components. There is hardly any increase for the Matlab routines, which is due to efficient vectorization, while the increase is close to linear for the C routines.

3. VAPOR-COMPRESSION CYCLE

In this section we describe a vapor-compression cycle (VCC) for the modeling of heat pumps or refrigerators. Furthermore, we present the effect of ambient conditions on the performance of a heat pump in order to emphasize the need for thermodynamically rigorous computation of the efficiency of heat pumps.

A heat pump is a reversed heat engine that transfers heat from a low temperature zone to one with a higher temperature using mechanical work for compression. Fig. 3 shows a schematic drawing of a VCC with a typical temperature-entropy diagram. The VCC consists of four steps. First the low pressure and low temperature refrigerant (point 1) is evaporated in a heat exchanger producing a saturated vapor (point 2). This saturated low pressure vapor is compressed isentropically by supplying work, W_c, in the compressor to produce a high temperature and high pressure vapor (point 3). Afterwards, heat is released in the condenser at constant pressure, producing a saturated liquid phase (point 4). Finally, the saturated liquid is expanded to its original pressure at isenthalpic conditions in a turbine or in a throttling valve (point 1). The coefficient of performance (COP) provides the overall energy efficiency of a VCC used for either heating, $\mathrm{COP}_{\mathrm{heat}}$, or cooling, $\mathrm{COP}_{\mathrm{cool}}$. These COPs are defined as

$$\mathrm{COP}_{\mathrm{heat}} = \frac{h_3 - h_4}{h_3 - h_2}, \tag{1a}$$

$$\mathrm{COP}_{\mathrm{cool}} = \frac{h_2 - h_1}{h_3 - h_2}, \tag{1b}$$

where h_1, h_2, h_3, and h_4 are the enthalpies of the refrigerant in the four points in the cycle. At nominal operating conditions, a COP of a heat pump is often set to 3. This indicates that the extracted heat is 3 times the energy input to the compressor. However, the COP is a nonlinear function of the evaporation temperature, condensation temperature, the active load, and the isentropic efficiency of the compressor. Therefore, thermodynamically correct and accurate modeling of this unit is necessary for reliably determining the performance of a VCC and for realistic optimal control of processes with integrated heat pumps. The dynamics of VCCs are in general much faster than the dynamics of buildings and industrial processes (Halvgaard et al., 2012; Hovgaard et al., 2013; Jensen and Skogestad, 2007; Svensson, 1996; Zhao et al., 2003). Therefore, we implement a static model of a heat pump. This model is based