ROBUST AND COMPUTATIONALLY EFFICIENT DYNAMIC SIMULATION OF ORC SYSTEMS: THE THERMOCYCLE MODELICA LIBRARY

S. Quoilin*, A. Desideri, I. Bell, J. Wronski, V. Lemort

University of Liege
Energy Systems Research Unit
Chemin des Chevreuils, 7, 4000 Liege, Belgium
e-mail: squoilin@ulg.ac.be
web page: www.labothap.ulg.ac.be

EXTENDED ABSTRACT

INTRODUCTION

The ThermoCycle library, an open-source library for dynamic modeling of ORC systems, has been recently developed in the Modelica language and is presented in this paper. Special attention has been paid to robustness and to simulation speed. Dynamic simulations are indeed often limited by numerical constraints and failures, either during initialization or during integration. Furthermore, the use of complex equations of state (EOS) to compute thermodynamic properties dramatically decreases the simulation speed. In this paper, the different numerical methods developed to overcome these limitations are presented and discussed and the proposed models are then benchmarked against alternative simulation tools.

MODELICA LIBRARIES FOR THERMODYNAMIC CYCLES

The Modelica language is well adapted to the formulation of thermo-flow problems, mainly because it is an a-causal language that allows interconnecting the models in a "physical" way (Casella et al., 2007). A number of libraries are available to model steam or gas cycles (e.g. ThermoSysPro, Power Plants, etc.), but few are able to handle the fluids used in ORC systems. Thermodynamic properties of (moist) air and water are indeed well known and implemented in most simulation tools while the ones of organic fluids require complex equations of state available only in external libraries such as FluidProp (Colonna and van der Stelt, 2004), Refprop (Lemmon et al., 2010) or CoolProp (Bell et al., 2013). Three Modelica libraries available for the simulation of ORC systems are analyzed in this section.

Modelica.Fluid and Modelica.Media

Modelica.Fluid provides zero- and one-dimensional thermo-fluid components. It is based on Modelica.Media, part of the Modelica Standard Library, to compute fluid properties. In the Modelica.Fluid library the energy balance equations, implemented in the control volumes, depend on a comprehensive set of fluid property derivatives that cannot be provided by external libraries such as ExternalMedia.

TIL and TILMedia

TIL is a commercial library for steady-state and transient simulation of thermodynamic systems (TLK Thermo GmbH, 2013). The thermodynamic properties are obtained through TILMedia, an interface between Modelica and Refprop that also includes custom high performance EOS for selected working fluids. The library comprises several models for thermodynamic systems (e.g. heat exchangers, expanders, pumps, etc.).

ThermoPower and ExternalMedia

The ThermoPower library has proven to be well suited for the modeling and the validation of ORC systems (Casella et al., 2013). It is based on the ExternalMedia library, an interface between Modelica and FluidProp. ThermoPower and ExternalMedia are open-source, FluidProp is freely available but not open-source.

THE THERMOCYCLE MODELICA LIBRARY

The ThermoCycle library aims at providing a robust framework to model thermal systems, including ORC systems. The goal is to provide a fully open-source integrated solution going from thermodynamic properties, using CoolProp (Bell et al., 2013), to the simulation of complex systems with their control strategy. The interface between ThermoCycle and CoolProp is ensured by the CoolProp2Modelica library, which is based on a modified version of the ExternalMedia library.

Available components

The library provides a set of components, most of which have been validated against experimental data, that can be used to model thermodynamic cycles: 1D-Flow models for compressible and incompressible fluids, finite volumes heat exchangers, moving boundaries heat-exchangers based on (Kærn, 2011), simplified expander models and detailed ones based on (Lemort et al., 2009), valve and pressure drop models, solar collector models, tank and pump models plus practical examples of ORC cycle simulators for various applications, including examples of PID-based and linear MPC control systems.

NUMERICAL METHODS

The different numerical methods developed to ensure robustness and simulation speed are hereunder described.

Chattering in finite volume two-phase flow models

The phenomenon of chattering may occur when discontinuities in the model variables are present (Bonilla et al., 2012). This phenomenon can lead the computed variables to exceed acceptable boundaries, causing simulation failures. In a discretized heat exchanger model, the main discontinuity is often the density derivative on the liquid saturation curve. Simulation failure occurs if the cell-generated, non-physical flow rate due to this discontinuity is of the same order of magnitude as the working fluid flow rate in the cycle. Therefore, a numerical stability criteria can be expressed as follows:

$$\dot{M}_{su} \gg \frac{V}{N} \cdot \frac{d\rho_i}{dt} = \frac{V}{N} \cdot \left[\left.\frac{\partial \rho_i}{\partial h}\right|_p \cdot \frac{dh_i}{dt} + \left.\frac{\partial \rho_i}{\partial p}\right|_h \cdot \frac{dp}{dt} \right] \tag{1}$$

Chattering and simulations failures are likely if (1) the number of cells (N) is low, (2) the cycle working fluid flow rate ($\dot{M}_{su}$) is low, (3) the heat exchanger internal volume (V) is high, (4) the working conditions are highly transient (i.e. $\frac{dp}{dt}$ and $\frac{dh}{dt}$ are high). The variables $\frac{\partial \rho_i}{\partial h}$ and $\frac{\partial \rho_i}{\partial p}$ are thermodynamic properties of the working fluid and are discontinuous at the saturation lines, especially at the transition between liquid and two phase, where chattering and simulation failures usually occur. Different numerical methods are implemented to overcome this issue: (I) truncation of the $\frac{\partial \rho_i}{\partial h}$ and $\frac{\partial \rho_i}{\partial p}$ partial derivatives, (II) filtering the density derivative $\frac{d\rho}{dt}$ using a first-order filter, (III) imposing a constant node flow rate and reporting the mass accumulation terms on the outlet flow rate, (IV) smoothing of partial derivatives using a spline function at the transition from liquid to two-phase state, (V) ensuring continuous first partial derivatives of the density function. It is noteworthy that the two last methods are implemented in the library of the thermodynamic properties. This was possible since the CoolProp library is open-source and tightly integrated with ThermoCycle.
A comparison of these different methods, based on the simulation of an heat exchanger with an high number of cells, in terms of simulation speed, simulation accuracy and mass and energy imbalance shows that adopting the proposed methods can dramatically improve the simulation performances at the expense of a small decrease of the accuracy. The maximum error on the energy balance varies from 0.1 % to 0.3 % depending on the selected method.

Initialization issues
The convergence of the Newton Solver during initialization is a key challenge when modeling complex system. Several strategies have been developed, such as the *homotopy* method (Sielemann et al., 2011). A different approach has been selected in ThermoCycle: the system is initialized on a simplified system of equations, and the more complex non-linear equations (such as the computation of the heat transfer coefficients as a function of mass flow) are activated one by one during integration using a purposely designed *initialization* component.

Simulation speed
As stated above, simulation speed in ORC simulators mainly depends on the computational-efficiency of the external thermodynamic library. Special care has been taken to optimize each property call and to limit double calls. In order to further improve the simulation speed an interpolation method has been implemented in CoolProp: the interpolation tables are built at the beginning of the simulation, which takes between 2s and 10s, and all the properties are further obtained by a second-order interpolation. The method presents the advantage of being fully transparent for the user, who just needs to activate a flag in the Modelica property call (Bell et al., 2013). A speed benchmark run on an ORC model with control system shows that the model with CoolProp is about

40 % faster than with TILMedia and 10 times faster if the interpolation method is used.

ACKNOWLEDGEMENTS

Some results presented in this paper have been obtained within the frame of the IWT SBO-110006 project The Next Generation Organic Rankine Cycles (www.orcnext.be), funded by the Institute for the Promotion and Innovation by Science and Technology in Flanders. This financial support is gratefully acknowledged.

LITERATURE

I. H. Bell, S. Quoillin, J. Wronski, and V. Lemort. Coolprop: An open-source reference-quality thermophysical property library. In *submitted abstract to ASME-ORC 2013 – 2nd International Seminar on ORC Power Systems*, 2013.

J. Bonilla, L. Yebra, and S. Dormido. Chattering in dynamic mathematical two-phase flow models. *Applied Mathematical Modelling*, 36(5):2067–2081, 2012.

F. Casella, J. van Putten, and P. Colonna. Dynamic simulation of a biomass-fired steam power plant: A comparison between causal and a-causal modular modeling IMECE2007-41091. In *Proceedings of the International Mechanical Engineering Congress*, volume 6, pages 205–216, 2007.

F. Casella, T. Mathijssen, P. Colonna, and J. van Buijtenen. Dynamic modeling of organic rankine cycle power systems. *Journal of Engineering for Gas Turbines and Power*, 135(4):042310, Mar. 2013.

P. Colonna and T. P. van der Stelt. *FluidProp: a program for the estimation of thermo physical properties of fluids*. Energy Technology Section, Delft University of Technology, 2004.

M. R. Kærn. *Analysis of Flow Maldistribution in Fin-and-tube Evaporators for Residential Air-conditioning Systems*. Phd thesis, Technical University of Denmark, 2011.

E. Lemmon, M. Huber, and M. McLinden. *NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP*. National Institute of Standards and Technology, Boulder, Colorado, 2010.

V. Lemort, S. Quoilin, C. Cuevas, and J. Lebrun. Testing and modeling a scroll expander integrated into an organic rankine cycle. *Applied Thermal Engineering*, 29(14-15): 3094–3102, 2009.

M. Sielemann, F. Casella, M. Otter, C. Clauß, J. Eborn, S. E. Mattsson, and H. Olsson. Robust initialization of differential-algebraic equations using homotopy. In *Proceedings of the 8th Modelica Conference*, pages 21–22, Dresden, 2011.

TLK Thermo GmbH. TIL Suite - Simulates Thermal Systems, April 4th 2013. URL `http://www.tlk-thermo.com`.