A new IPSEpro® library for the simulation of binary mixtures of real fluids in power cycle analysis

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Abstract
Increasing efforts to produce power from renewable resources and improve the efficiency of current industrial processes have turned the spotlight on organic Rankine cycles (ORC). The use of refrigerant mixtures in these cycles offers a wide range of possibilities for fluid selection and optimization. Moreover, zeotropic mixtures are reported to yield better cycle performances due to their better thermal match with the source and sink streams. In this work a new IPSEpro® library for the simulation of power cycles using binary mixtures was developed. With this library the working fluid can be defined as the mixture of any pair of suitable fluids contained in the Refprop database.

Keywords: fluid mixtures , IPSEpro, ORC, Refprop.

Introduction

The use of organic Rankine cycles (ORC) is becoming of increasing interest because of their suitability for power production from low heat sources (Bao & Zhao, 2013; Hung, Shai, & Wang, 1997). Low-temperature energy sources can be found not only among renewable energy systems such as geothermal wells, solar concentration systems or biomass combustion plants, but also in the waste heat streams from industrial processes consuming conventional fuels. Therefore, the use of ORC can play an important role, not only in the introduction of renewable energy, but also in the improvement of the efficiency of current energy demanders.

One of the advantages of ORC is the great availability of organic working fluids which allows for the selection of the media that better optimizes the overall cycle energy performance. However, the beneficial thermodynamic behavior of some organic fluids already in use in refrigeration systems and heat pumps, run counter their environmental or safety characteristics. In this context refrigerant blends appeared as replacement media for these systems (Didion & Bivens, 1990). In addition, zeotropic mixtures are reported to increase the efficiency of these systems due to a better thermal match of the fluid with the source and sink streams (Angelino, Colonna, & Paliano, 1998).

Although refrigerant mixtures have been extensively used in refrigeration schemes, their presence in thermal power generation is still limited (Chys, van den Broek, Vanslambrouck, & De Paepe, 2012; Rajapaksha, 2007). As a consequence, many of today's power plant process simulators cannot deal with the use of mixtures as working fluids, or just with a limited amount of options.

In this work we present the implementation of a library for the use of binary mixtures of fluids in the process simulator IPSEpro®. Thermophysical properties of the mixtures were estimated by calling the real fluid equations of state of the Refprop subroutines (E.W. Lemmon, Huber, & McLinden, 2013). As a result, binary mixtures containing any combination of suitable fluids from the Refprop database can be used for thermodynamic analysis with the IPSEpro® process simulator.

IPSEpro® process simulator

IPSEpro® (SimTech, 2013) is a commercial software for process modelling developed by SimTech of Graz, Austria. This software can be used for both steady-state and off-design analyses of thermal power systems. The main characteristic of IPSEpro® is that it is an open equation modeling environment, which means that the engineering equations are not part of the source code, and therefore can be extended by the users, conferring greater flexibility to adapt and create models to satisfy each user needs.

IPSEpro® provides a graphic Process Simulation Environment (PSE) for the construction of the process model by linking units (which for thermal power cycles represent the models of the cycle components) through connections (which correspond to the heat transfer fluid streams). Input operational conditions and algebraic equations can be introduced as well in this environment. Moreover, both standard predefined and user-defined units can be used to build process models. The user-defined models can be coded in the Model Development Kit (MDK). Once the process scheme is set, the PSE solver core resolves the system of equations and variables by using the Newton-Raphson algorithm for numerical root-finding. This method consists of a series of iterations to estimate the system variables values, as expressed in (1). It starts from seed values set by the user, and stops when a certain degree of residual value between consecutive iterative values is achieved.

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \qquad (1)$$

Although IPSEpro® is conceived as a flexible simulation platform in which the user can create new models by using the MDK, the features of the code editor cannot handle complex algorithms. However, the use of Dynamic Link Libraries (DLL) overcomes this limitation by providing access to external functions. DLL contain a set of functions defined by the user that can be called from the MDK to be used both in the connection properties or the unit models.

There are several available commercial libraries for IPSEpro® that consist of a set of predefined models and a corresponding DLL that contains the needed external functions. Among these libraries Frigo_Lib® and LTP_Lib® are intended for simulation of thermal compression systems and low-temperature processes, respectively. Both libraries support thus the modelling of organic Rankine cycles using pure fluids or predefined mixtures as working fluids. In addition, the later provides the capability to analyze Kalina cycles based on ammonia-water mixtures and supercritical CO_2 cycles. Both libraries are in compliance with the state-of-the-art equations of state for the calculation of thermodynamic properties of the fluids. Nevertheless, none of these libraries allow the study of user-defined mixtures. Only ammonia-water mixtures, or Ideal gas mixtures of components commonly present in exhaust gases can be studied.

Several authors have worked on the implementation of libraries to extend the capabilities of IPSEpro®. For instance, Ji et al. (Ji, Jonsson, Yan, & Processes, n.d.) developed a real thermodynamic property model for humid gas for its use in humidified gas turbine processes. In addition Thorbergsson et al. (Thorbergsson, Grönstedt, & Robinson, 2013) implemented a library for the use of real fluid mixtures in their simulations for turbomachinery design. The developed library supported the estimation of multicomponent mixtures containing Ar, CO_2, H_2O, N_2 and O_2. Moreover, Dejfors and Svedberg (Dejfors & Svedberg, 1999) developed an interface to connect IPSEpro® with predefined subroutines for the estimation of the thermodynamic properties of ammonia-water mixtures.
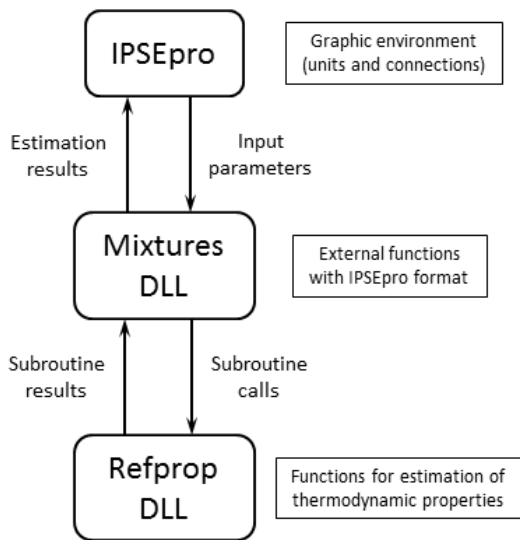
Figure 1. IPSEpro® and the Refprop DLL link. Basic structure of the connection between IPSEpro® and the Refprop DLL through the newly developed DLL for mixtures.

As we aim at a broad research on the use of different fluid blends in thermal power systems it was considered necessary to develop a library for the simulation of systems using binary mixtures as working media in IPSEpro®.

Implementation of the library for binary mixtures

In order to be able to study binary mixtures containing any suitable pair of fluids included in the Refprop database, a new library was developed. This library makes use of extern functions allocated in a Dynamic Link Library (DLL) that call the NIST Refprop subroutines.

The DLL was coded for IPSEpro® version 5.1. in the programming language C++ and compiled with Microsoft Visual Studio 2010 Professional design environment. MDK was used to create the new connections, global variables and models for the mixtures library. Figure 1 depicts the principal structure of the data link between

IPSEpro® and the Refprop DLL through the use of the newly developed DLL for mixtures.

In this way, the DLL for mixtures acts as an intermediary DLL that contains the functions necessary to call the Refprop subroutines. The DLL is necessary to establish a connection between the two different formats of the functions required by IPSEpro® and Refprop. Once the DLL is called it becomes active and part of the program.

The range of application of the DLL for the calculation of the thermophysical properties is that of the Refprop subroutines for each mixture, and covers the liquid and gas phases, and the two-phase region. Some combination of mixtures will likely yield calculation errors because of a lack of interaction parameters in the Refprop model. Also, it is important to notice that for some cases the mixture parameters are estimated values and therefore could affect the accuracy of the thermodynamic properties used in the model (Eric W Lemmon & McLinden, 2013). The user can select easily both fluids through their identification numbers and select the composition of the mixture by setting the mole fraction of the first component. The computational time achieved with the implemented DLL was found to be only slightly longer than that of the commercial libraries mentioned in the previous section and is of the same order of magnitude (few seconds for an ORC model).

Table 1 contains all the functions defined in the new DLL for the calculation of the thermodynamic properties of binary mixtures. It must be pointed out that for each function, its first derivative respect to each of the independent variables must be defined, according to the algorithm in (1). In this DLL we defined the derivatives by using the five-point stencil method in one dimension (Hoffman, 2001), as expressed in (2).

Table 1. External functions defined in the new DLL for the calculation of the mixtures properties.

Functions with p and h as independent variables	Functions with p and T as independent variables	Functions with T and v as independent variables
$T\left(p,h,Fluid1,Fluid2,x_{Fluid1}\right)$	$h\left(p,T,Fluid1,Fluid2,x_{Fluid1}\right)$	$h\left(T,v,Fluid1,Fluid2,x_{Fluid1}\right)$
$s\left(p,h,Fluid1,Fluid2,x_{Fluid1}\right)$	$s\left(p,T,Fluid1,Fluid2,x_{Fluid1}\right)$	$s\left(T,v,Fluid1,Fluid2,x_{Fluid1}\right)$
$v\left(p,h,Fluid1,Fluid2,x_{Fluid1}\right)$	$v\left(p,T,Fluid1,Fluid2,x_{Fluid1}\right)$	$p\left(T,v,Fluid1,Fluid2,x_{Fluid1}\right)$
$q\left(p,h,Fluid1,Fluid2,x_{Fluid1}\right)$	$q\left(p,T,Fluid1,Fluid2,x_{Fluid1}\right)$	$q\left(T,v,Fluid1,Fluid2,x_{Fluid1}\right)$
Functions with p and q as independent variables	**Functions for the saturated states**	
$h\left(p,q,Fluid1,Fluid2,x_{Fluid1}\right)$	$h_{SL}\left(T,Fluid1,Fluid2,x_{Fluid1}\right)$	
$T\left(p,q,Fluid1,Fluid2,x_{Fluid1}\right)$	$h_{SV}\left(T,Fluid1,Fluid2,x_{Fluid1}\right)$	
$s\left(p,q,Fluid1,Fluid2,x_{Fluid1}\right)$		

$$f'(x) \approx \frac{-f(x+2\varepsilon)+8f(x+\varepsilon)-8f(x-\varepsilon)}{12\varepsilon} +$$
$$+\frac{f(x-2\varepsilon)}{12\varepsilon} \tag{2}$$

Here $f'(x)$ refers to the partial derivative of the function f respect to the independent variable x, and ε is the machine epsilon. Models of the main components for ORC simulation were implemented by duplicating the existing ones in the provided library and adapting them for their use with the fluids mixtures.
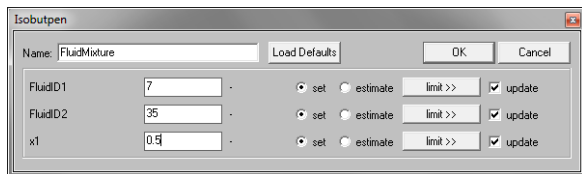
Figure 2. Window for the selection of the mixture components and composition for a global variable.

The great advantage of this new library is that both components of the studied mixture can be chosen from among 120 different fluids. The mixtures variables (i.e. the mixture components and composition) can be easily modified in the PSE, as shown in Figure 2, but also through the COM interface module from any client application, such as Matlab. This feature makes it

easier and faster to perform cycle analysis over a wide range of variations of the mixture properties or components for the same process model. An additional possibility of the new library is that it can be also used to simulate pure fluids by just setting equal mixture components and the fluid mole fraction $x=1$. Moreover, this library can be combined with other commercial or user-defined libraries and their components, if desired.
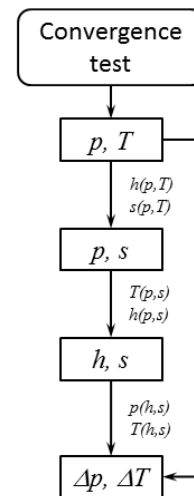
Figure 3. Convergence test flow chart

The convergence of the calculations performed with the new DLL was tested by applying the loop depicted in Figure 3. Magnitudes in boxes represent the independent variables used on

each step and functions on the side represent the dependent variables. Although none of the functions defined in Table 1 have the entropy as an independent variable, a combination of them is used in the solving procedure to estimate the magnitudes from *(p,s)* and *(h,s)* values. The error in pressure and temperature after the loop was found to be less than 0.01%, which turned out to be of the same order of magnitude as that obtained after applying the commercial library for a pure substance.

The main feature of this library is that with just one DLL it is possible to access any binary mixture by just changing the components identification numbers. This permits performing studies over a wide range of mixtures and for different compositions in little computational time. Another advantage is that it is possible to work with different compositions of a binary mixture in the same process scheme, thus allowing us to model systems in which stream compositions changes, as it happens, for instance, in systems using absorption or distillation processes.

Example of use

As an example of the use of the new library for binary mixtures, a scanning of different mixtures and compositions was run for a simple saturated ORC without regeneration, with a source temperature of 350 K and a sink temperature of 280 K. Mass flow rates of the cycle and sink were optimized for the minimum mean temperature difference in both heat exchangers. The studied binary mixtures contained the same components as the following predefined binary mixtures of the Refprop database: R415A, R421A, R500 and R431A. However the mole fraction of the components for each mixture was varied over the whole supported composition range. Figure 4 depicts the overall energy efficiency of the ORC for each mixture versus the mole fraction of the first component. Red dots represent the efficiency and composition for the mentioned predefined mixtures. It can be observed that by studying a wide range of compositions for a mixture, rather than being constrained to a fixed

one, it is possible to optimize the composition of the mixture according to specific parameters. In this example, it would be possible to choose a mixture composition with higher cycle efficiency than that given by the predefined mixtures, or to optimize it according to other safety (flammability, health) or environmental restrictions. Hence we prove the power and utility of our new DLL to perform an extensive research on the use of fluids blends in power cycles.
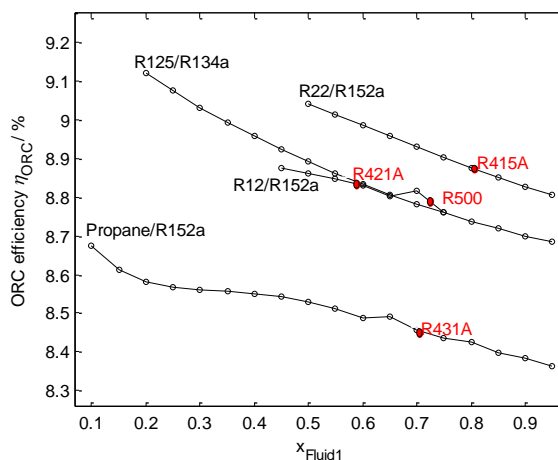
Figure 4. ORC efficiency for different mixtures vs. composition. Mole fraction of the first component of the mixture is in axis x. Red dots depict the predefined refrigerant mixtures corresponding for those components and composition.

Conclusions

A DLL coded in C++ was developed to integrate the estimation of the thermodynamic properties of binary mixtures of Refprop into the process simulator IPSEpro®. The DLL contains the functions required by the IPSEpro® solver to perform the thermodynamic analysis of the process. Main components of thermal power systems were modelled for their use in the design of power cycles using mixtures as working fluids. The DLL calculation time was found to be of the same order of magnitude of the existing libraries for real pure components simulation in IPSEpro®.

Nomenclature

h	Enthalpy
p	Pressure
s	Entropy
q	Vapor quality
T	Temperature
v	Specific volume
x	Mole fraction
DLL	Dynamic link library
Fluid1, Fluid2	Mixture components
MDK	Model development kit
ORC	Organic Rankine cycles
PSE	Process simulation environment
SL	Saturated liquid
SV	Saturated vapor

References

Angelino, G., Colonna, P., & Paliano, D. I. (1998). Multicoponent working fluids for Organic Rankine Cycles (ORCs), *23*(6), 449–463.

Bao, J., & Zhao, L. (2013). A review of working fluid and expander selections for organic Rankine cycle. *Renewable and Sustainable Energy Reviews*, *24*, 325–342. doi:10.1016/j.rser.2013.03.040

Chys, M., van den Broek, M., Vanslambrouck, B., & De Paepe, M. (2012). Potential of zeotropic mixtures as working fluids in organic Rankine cycles. *Energy*, *44*(1), 623–632. doi:10.1016/j.energy.2012.05.030

Dejfors, C., & Svedberg, G. (1999). Second Law Analysis of Ammonia-Water Power Cycle for Direct-fired Cogeneration Application, *2*(3), 125–131.

Didion, D. a., & Bivens, D. B. (1990). Role of refrigerant mixtures as alternatives to CFCs. *International Journal of Refrigeration*, *13*(3), 163–175. doi:10.1016/0140-7007(90)90071-4

Hoffman, J. D. (2001). *Numerical methods for engineers and scientists.pdf* (Second Edi.).

Hung, T. C., Shai, T. Y., & Wang, S. K. (1997). A review of organic Rankine cycles (ORCs) for the recovery of low-grade waste heat, *22*(7), 661–667.

Ji, X., Jonsson, M., Yan, J., & Processes, E. (n.d.). Implementation of a real thermodynamic property model in IPSEpro, (Dll).

Lemmon, E. W., Huber, M. L., & McLinden, M. O. (2013). NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 9.1. *National Institute of Standards and Technology*. Gaithersburg,: National Institute of Standards and Technology, Standard Reference Data Program.

Lemmon, E. W., & McLinden, M. O. (2013). Method for estimating mixture equation of state parameters. *Magnesium Research : Official Organ of the International Society for the Development of Research on Magnesium*. doi:10.1684/mrh.2013.0347

Rajapaksha, L. (2007). Influence of special attributes of zeotropic refrigerant mixtures on design and operation of vapour compression refrigeration and heat pump systems. *Energy Conversion and Management*, *48*(2), 539–545. doi:10.1016/j.enconman.2006.06.001

SimTech. (2013). IPSEpro Process Simulator. Program Modules and Model Libraries, SimTech.

Thorbergsson, E., Grönstedt, T., & Robinson, C. (2013). Integration of fluid thermodynamic and transport properties conceptual turbomachinery design. In *Proceedings of ASME Turbo Expo 2013: Turbine Technical Conference and Exposition* (pp. 1–8).