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David H. Richardson
Reinhard Radermacher

Vikrant Aute
Reinhard Radermacher

Jonathan Winkler
Reinhard Radermacher

NUMERICAL CHALLENGES IN SIMULATION OF A GENERALIZED VAPOR COMPRESSION REFRIGERATION SYSTEM

David H. Richardson*, Vikrant Aute, Jonathan Winkler and Reinhard Radermacher

University of Maryland
Department of Mechanical Engineering
University of Maryland College Park, Maryland 20742, USA
E-Mail: dhr@glue.umd.edu, vikrant@glue.umd.edu, jwinkler@glue.umd.edu, rader@glue.umd.edu
*Author of Correspondence

ABSTRACT

VapCyc is a vapor compression refrigeration simulation tool which features charge management and component inter-changeability. In addition to the four basic cycle components, additional components, such as pipes, bypass valves and various auxiliary heat exchangers can be added to the system at run-time, rather than design time, making the simulation very user-friendly. The simulation is achieved through the solution of the system level conservation laws of mass and energy, which are satisfied through the evaluation of the performance relations of individual component models. This simulation technique presents numerical challenges. This paper presents the system level conservation laws and addresses the numerical challenges of convergence criteria, as well as equation and variable scaling. In addition, a methodology of estimating the solution over a wide range of refrigeration applications and refrigerants, to assist the numeric solver is developed.

1. INTRODUCTION

Previously, VapCyc was presented as a tool for vapor compression refrigeration system simulation and optimization by Richardson *et al*. (2002). VapCyc is a simulation tool which is limited in scope to a vapor compression refrigeration system, but maintains generality through interchangeable component models as well as the ability to add additional components to the system.

Generality is utilized in VapCyc for flexibility of system configuration as well as for the capability to simulate systems composed of component models which may be authored by any number of sources. When multiple sources are to be used, a set of standards must be developed for components, such that the VapCyc equation solver can accomplish its numeric goals for the simulation.

Two main elements of the component standard directly affect system level convergence tolerance as well as an initial estimate for the VapCyc solution routine.

This paper details the basic tolerance relations between components and the system level conservation equations. Also, a concept of a system context is presented. The context is specified to both the system and the components. Via the context the system and components can test compatibility and formulate an initial guess for the VapCyc solution routines.

2. VAPCYC REVIEW

A review of the VapCyc modeling concept is presented here to explicitly present the data structures and modeling equations which characterize the simulation. The data structures are components, ports, and junctions, while the modeling equations represent the system level mass, momentum, and energy conservation equations.

The VapCyc simulation is described with three main data structures for use in energy system simulation; namely, *components, ports* and *junctions*. Components, meaning the refrigeration system components, are modeled as black box objects interacting with one another via a working fluid, through a series of ports and junctions, and possibly with their environment.

2.1 Components

Components are represented by appropriate engineering models which themselves must satisfy all physical laws. A fluid flow enters or leaves a component through a port, which in turn communicates with a junction. Through this junction the fluid flow allows two or more components to communicate with one another.

Figure 1 illustrates a typical "black box" component and a detailed "black box" component. In this case, the component to be simulated is a combination of two compressors and an inter-cooler. This component communicates with its environment through work and heat transfer, and communicates with two other system components through its two ports and their respective junctions.

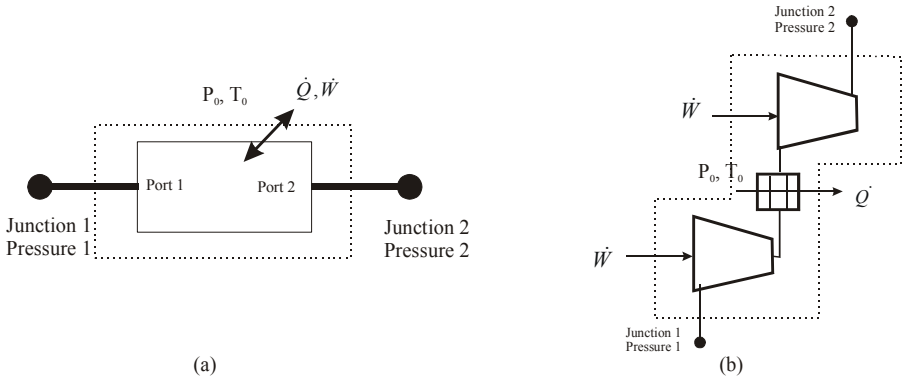


Figure 1: A black box representation a system component

The "black box" approach is used to generalize the fixed vapor compression system configuration to one in which the individual components themselves *are allowed* to have "non-traditional" work and heat transfer interactions with the environment. Examples would be a turbine expander, rather than the traditional expansion valve, or the compressor configuration shown in figure 1b.

2.2 Ports

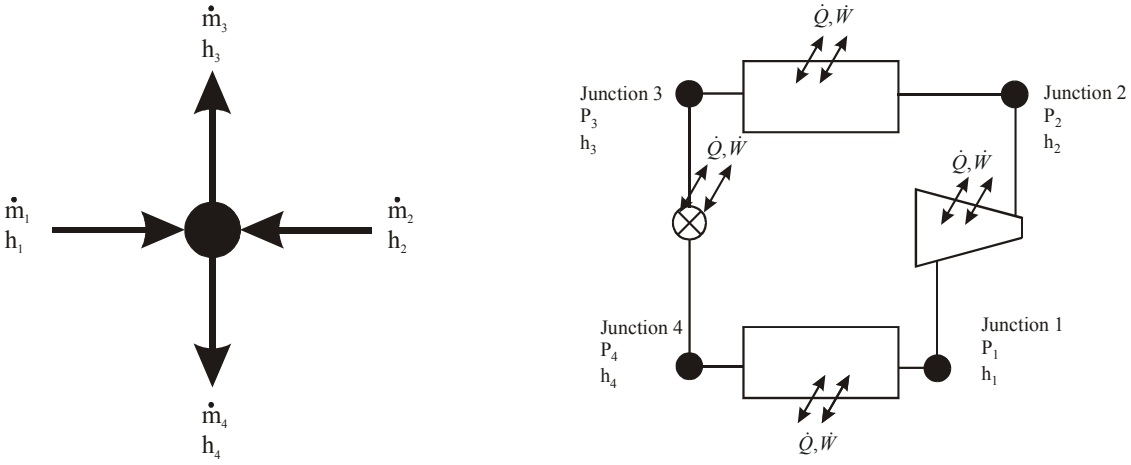
Ports are a component's interface with other components in the system where fluid flow is the mechanism of energy transport. The fluid flow through a port has a distinct flow rate and energy state, defined by the thermodynamic equation of state and any other energy contribution accounted for in the system simulation. Additional energy contributions may include (but are not limited to) chemical energy, such as that of a fluid flowing through an inlet valve to a combustion chamber, kinetic energy and electrical current.

2.3 Junctions

Junctions are infinitesimal points which allow for interaction of the components, through their ports, with the "system". In this context, the system refers to each component and its ports along the fluid flow path. The fluid flow path is any part of the system which the working fluid may make contact with. Examples of a fluid flow path are the sealed system of a vapor compression refrigeration system, the open system of a heat exchanger, or the natural gas pipeline of a community.

(a) (b)

Figure 2a illustrates a VapCyc system junction. The junction has a distinct value for its pressure, which is identical at each port connected to the junction. The mass flow rates ($\dot{m}_1, \dot{m}_2, \dot{m}_3, \dot{m}_4$) and direction of the flow at each port (in or out) are determined by the solution of the component's model for the given boundary conditions.



(a) (b)

Figure 2: A VapCyc Diagrams (a) VapCyc Junction, (b) Simple Refrigeration Cycle

The fluid flows entering a junction may have different specific enthalpies. Since the junctions do not contain any process for separating the fluid into different states, it is concluded that all flows leaving the junction have the same specific enthalpy. This enthalpy value for the junction is called its *mixing enthalpy*.

2.4 Conservation Equations

The pressure of each port connected to a junction is identical; therefore there are N_J (number of junctions) unknown pressures for the simulation. Each port may have a unique value for enthalpy and mass flow, leaving 2 N_p (number of ports) unknown variables to resolve the simulation. The system must solve for a total of 2 N_p + N_J unknown variables. The components supply mass flow rate and enthalpy for each outlet port, removing 2 $N_{p,out}$ equations. Therefore the total number of independent variables to be solved for are 2 N_p + N_J - 2 $N_{p,out}$. For this particular system this becomes (16 + 4 – 8). The independent variables are 4 junction pressures and 4 junction mixture enthalpies.

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The governing equations of *conservation of mass* and *conservation of energy* at the junction level each provide $2N_J$ equations.

Conservation of mass at each junction, J, provides four mass balance equations.

$$\sum_{p=1}^{Nports} \dot{m}_p = 0 \tag{1}$$

Conservation of energy at each junction, J, provides four energy balance equations. These energy balance equations can be manipulated into a form explicit in the unknown mixing enthalpy of the junction.

$$\sum_{pi=1}^{Nports,Inlet} \dot{m}_{pi} h_p - \sum_{po=1}^{Nports,Outlet} \dot{m}_{po} h_{po} = 0$$

or, since there is only one mixture enthalpy, h_o (2)

$$\frac{\sum_{pi=1}^{Nports,Inlet} \dot{m}_{pi} h_p}{\sum_{po=1}^{Nports,Outlet} \dot{m}_{po}} = h_{po}$$

Figure 2b illustrates a schematic of the simple fixed configuration vapor compression refrigeration system simulated by VapCyc. Using the previously identified structures, namely components, ports, and junctions, the proposed system has four components, with a total of eight ports connected at four junctions. Assuming steady state, this system simulation is considered solved when the thermodynamic state is known at each of the four junctions, and conservation laws *for the system* are obeyed.[1]

In closed systems, such as the basic vapor compression refrigeration systems, mass must be accounted for at all operating points in each of the components. A change in system boundary conditions (via the components) changes the operating point of the system, but not the system charge. For the closed system the junction mass flow rates are no longer independent. A mass balance over each junction results in a redundant equation, thus one junction mass balance must be removed. However, the number of system variables in the simulation remains the same. A mass balance over the entire system provides the equation necessary to close the system of equations.

$$Charge_{System} = \sum_{i=1}^{NComponents} Charge_i \tag{3}$$

This implies that two independent thermo-physical properties, such as pressure and specific enthalpy, at each junction in the system, will define the system's operating point such that mass and energy are conserved for the system. For this system, this results in a total number of eight unknowns.

3. UNCERTAINTY ISSUES IN SIMULATION

Using a finite number of bytes to approximate a real number introduces an inherent error to any simulation. This inherent error is reduced if all calculations are resolved to machine precision in all simulation programs. However, this degree of resolution is not practical from either a programming or a simulation run time perspective.

Energy system simulations deal with variables of vastly different orders of magnitude; examples include mass flow rate, pressure, enthalpy, viscosity, heat transfer coefficients, energy transfer and Reynolds number. Table 1 shows these variables, with typical orders of magnitude when standard SI units are utilized.

Table 1: Common Energy System Variables

Energy System Variable	SI Unit	Order of Magnitude
Mass flow rate	kg/s	O(1)
Pressure	Pa	$O(10^6)$
Specific Enthalpy	J/kg	$O(10^6)$
Viscosity	kg/m-s	$O(10^{-5})$
Heat Transfer Coefficient	W/m²-K	$O(10^2\text{-}10^3)$
Energy Transfer	W	$O(1\text{-}10^5)$
Reynolds Number	-	$O(1\text{-}10^7)$

A generalized simulation technique must have generalized solution routines. These routines must be independent of the scale in which these equations operate; therefore a scaling analysis is imperative. Also, the generalized routines must have convergence criteria set for them. To adequately determine the convergence criterion for a given routine, an uncertainty analysis should be performed.

3.1 Uncertainty Inherent In Calculations

The VapCyc modeling equations of section 2.4 require a component to provide mass flow rate and thermodynamic outlet states when provided its boundary conditions. The VapCyc simulation solver then uses these values to resolve the conservation equations (1) - (3). A component using an equation which is explicit in mass flow has essentially no numeric uncertainty in its mass flow value. However, if the mass flow were calculated using an

[1] It is implicit that the components themselves satisfy their own conservation laws

iterative technique, which is required when a closed form expression does not exist, the calculation is only as certain as the resolution of the iteration. This is the precision of the calculation. To the junction conservation equations, this precision refers to the range of answers which may be expected for successive calculations with the same boundary conditions, but perhaps different calculation methods or initial guesses. The imprecision of component calculations can have repercussions on the simulation program calling upon them. In cases where the resolution of a component is larger than that required of the conservation equations, these equations may be difficult or impossible to solve.

3.2 Uncertainty of an iterative mass flow calculation

To demonstrate the point of uncertainty, take for example, the calculation of mass flow through an adiabatic tube. Using the Haaland expression for friction factor (Haaland, 1983),

$$\frac{1}{\sqrt{f}} = -1.8 \log\left[\frac{6.9}{\mathrm{Re}_d} + \left(\frac{\varepsilon/d}{3.7}\right)^{1.11}\right] \tag{4}$$

the mass flow can be determined from boundary conditions alone. However, the friction factor requires the Reynolds number, which requires the velocity, which requires the mass flow. The resulting system of equations to be solved is given by equations (4) and (5) (White, 1998). This system of equations can be resolved to a tolerance in mass flow of ε, which must be defined such that the routine is considered converged when $r \le \varepsilon$, where r represents the residual. This value ε is the precision, or uncertainty, for determining the mass flow using this method.

$$\begin{aligned} \Delta P &= f\rho\frac{L}{D}\frac{V^2}{2} \quad (a) \\ \dot{m} &= \frac{\pi}{4}D^2\rho V \quad (b) \\ \mathrm{Re}_d &= \frac{\rho V D}{\mu} \quad (c) \end{aligned} \tag{5}$$

3.3 Junction Uncertainty

A junction mass balance is re-written with uncertainty accounted for in the component mass flow as,

$$\sum_{p=1}^{Nports}(\dot{m}+\varepsilon)_p \le \varepsilon_{Junction,mass} \tag{6}$$

Equation (6) demonstrates that the uncertainty in a junction mass balance is a function of the number of connections to the junctions, as well as the uncertainty in the component uncertainties.

Similarly, the junction energy balance is re-written as

$$\frac{\sum_{pi=1}^{Nports,Inlet}(\dot{m}_i h+\varepsilon)_p}{\sum_{po=1}^{Nports,Outlet}(\dot{m}_o+\varepsilon)_p} - h_{po} \le \varepsilon_{Junction,energy} \tag{7}$$

A potential danger exists here when the enthalpy values from components are uncertain to a certain degree. The uncertainty in an energy flow is written as

$$\varepsilon_{p,\dot{m}h} = (\dot{m}\varepsilon_h)_p + (h\varepsilon_{\dot{m}})_p \tag{8}$$

Therefore the uncertainty of the junction energy is a function of not only the number of ports connected to the junction, but a functional relationship between the mass flow and enthalpy uncertainties.

3.4 Junction Scaling

The benefits of scaling the residual equations are readily available in numerical analysis texts, such as those given by Nash and Sofer (1996) and Press *et al*. (1999). The choice of scaling variables is problem specific. However, a generalized energy system simulation, as is utilized by VapCyc, has common thermo-physical properties and dependent variables.

Consider the case in which the dependent variables for the simulation are the mass flow and exit enthalpy at each component port, and the refrigerant charge within each component. The system independent variables are junction pressures and junction enthalpies.

The independent variables should be scaled with physically meaningful characteristic values. Each VapCyc simulation, regardless of system configuration always has the components of the basic cycle. It is therefore conceivable to use characteristic high and low values for pressure and enthalpy to scale the independent variables. Equation (9) offers possibilities for the scaled variables.

$$\begin{aligned} P_J^* &= \frac{P_J - P_{low}}{P_{high} - P_{low}} \\ h_J^* &= \frac{h_J - h_{low}}{h_{high} - h_{low}} \end{aligned} \tag{9}$$

The conservation equations should be scaled by characteristic value for the system dependent variables. Using

$$\begin{aligned} \overline{\dot{m}} &= \dot{m}_{compressor} \\ \overline{\dot{Q}} &= \overline{\dot{m}}\left(h_{high} - h_{low}\right) \\ \overline{Charge} &= Charge_{System} \end{aligned} \tag{10}$$

the junction conservation equations can be re-written as

$$\frac{\sum_{p=1}^{Nports} \dot{m}_p}{\overline{\dot{m}}_{Compl}} \le \varepsilon_{Junction,mass} \tag{11}$$

$$\frac{\dfrac{\sum_{pi=1}^{Nports,Inlet} \dot{m}_{pi} h_p}{\sum_{po=1}^{Nports,Outlet} \dot{m}_{po}} - h_{po}}{\overline{Q_{Evap}}} \le \varepsilon_{Junction,mass} \tag{12}$$

$$\frac{\sum_{i=1}^{NComponents} Charge_i - System\ Charge}{\overline{Charge}} \le \varepsilon_{Charge} \tag{13}$$

3.5 A System Context

How does one scale the variables and equations of a simulation when the result of the simulation is unknown? The answer to this question is found in the very "real life" concept of equipment rating.

Figure 3 shows rating points which vary with compressor application, as published in the ARI 540-99 standard.

Table 1. Standard Rating Conditions for Compressors and Compressor Units for Commercial Refrigeration Applications (Based on 95°F [35°C] Ambient Temperature)

Suction Dew Point Temperature		Compressor Type	Discharge Dew Point Temperature		Return Gas Temperature	
°F	°C		°F	°C	°F	°C
45	7.2	All	130	54.4	65	18.3
20	-6.7	All*	120	48.9	40/65*	4.4/18.3*
-10	-23.3	Hermetic	120	48.9	40	4.4
-25	-31.7	All*	105	40.6	40/65*	4.4/18.3*
-40	-40	All*	105	40.6	40/65*	4.4/18.3*

If air flow across the compressor is used to determine ratings, it shall be specified by the compressor manufacturer.
* For hermetic type compressors 40°F [4.4°C] return gas temperature shall be used.
For external drive and accessible hermetic type compressors 65°F [18.3°C] return gas temperature shall be used.

Figure 3: ARI 540-99 Rating Points for Compressors

Two compressors that may have similar capacity values as the ASHRAE high temperature rating point from figure 3,Figure 4, they may have very different capacities at a different ASHRAE rating point. Thus the standard effectively provides different contexts which can be applied to compressors, allowing the compressors performance at different operating points to be defined.

Using a context for each component in the system allows components to be compared to one another with respect to mass flow (capacity) and energy performance. Table 2 illustrates the high and low temperatures encountered in a standard vapor compression refrigeration cycle. These values along with a refrigerant, a degree of evaporator superheat, condenser subcooling and compressor discharge superheat allows for the calculation of the values in equation (9).

The components provide their performance values at the specified context. These performance values provide the necessary information to determine the scaling values referenced in equation (10), and also provide a good initial guess for the solution to the system. Comparing values of mass flow and exit energy states, a rough determination of component compatibility can be tested.

For example, if the low temperature refrigeration context is applied to a set of components designed for air-conditioning application, the components may no longer be suitably matched. The low suction pressure would likely result in a dramatically decreased capacity by the compressor and evaporator. The condenser context is not very different between the two applications, so the condenser and expansion device performance do not change much. The large discrepancy in nominal capacities between the components would serve as a warning that the simulation has contains poorly matched components and may not find an acceptable solution.

Table 2: VapCyc Contexts

Context	**Evaporating Temperature (°F/°C)**	**Condensing Temperature (°F/°C)**
Residential Air-Conditioning	45.0 / 7.2	130.0 / 54.4
Residential Heat Pump	30.0 / -1.1	110.0 / 43.3
High Temperature Refrigeration	20.0 / -6.7	120.0 / 48.9
Medium Temperature Refrigeration	-25.0 / -31.7	120.0 / 48.9
Low Temperature Refrigeration	-40.0 / -40.0	105.0 / 40.6

6. CONCLUSIONS

- Uncertainty in numeric calculations cannot be avoided. A generalized energy system, such as VapCyc must therefore establish standards for establishing convergence levels for components relative to the system level convergence specifications.
- The data structures of ports, junctions and components allows the uncertainty of a given system level conservation equation to be calculated, and thus a minimum convergence level for components to be determined.
- A generalized system solver does not have a priori knowledge of the components it contains. Utilizing component ratings, as are often used to publish catalog data for component performance allow a generalized solver and components to communicate on a fundamental level.
- This communication, obtained by evaluating components at a context specified by the system solver allows for a rough estimate of component compatibility, as well as a built in initial guess estimate.

NOMENCLATURE

d,D	diameter	(m)
f	friction factor	(-)
h	Enthalpy	(kJ/kg)
L	Length	(m)
$\dot{m}$	Mass flow rate	(kg/s)
N	Number	(-)
P	Pressure	(Pa)
$\dot{Q}$	Heat Transfer Rate	(W)
Re_d	Reynold's Number	(-)
T	Temperature	(K)
V	Velocity	(m/s)
$\dot{W}$	Power	(W)

Greek Letters

ε	relative roughness	(m)
ε	uncertainty	(kg/s, W)
ρ	density	(kg/m^3)
μ	dynamic viscosity	(Pa-s)

Subscripts

i	in
J	Junction
o	out
p	port
System	for system

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