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Consistent Initialization of System of Differential-Algebraic Equations for Dynamic Simulation of Centrifugal Chillers

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ABSTRACT

For simulation of centrifugal chiller system with differential algebraic equations (DAEs), consistent initial conditions are difficult to obtain due to the two-phase refrigerant cycle and the connections between several components. Existing rigorous initialization methods are generally not easy to apply and not suitable for the particular problem of centrifugal chiller simulation, such as the surge avoidance. In this paper, the transient model of a water-cooled centrifugal chiller is developed in Modelica with Dymola and the TLK/IfT Library (TIL). A new preprocessing scheme and a direct initialization method are proposed for the consistent initialization for centrifugal chiller. Simulation results have shown the effectiveness of the proposed modeling framework and the initialization method.

1. INTRODUCTION

For numerical simulation of thermo-fluid systems which often include sets of differential algebraic equations (DAEs), consistent initialization is often difficult to obtain (Ascher and Petzold 1998). The procedure for solving DAE systems typically includes two steps. The first step is to search and obtain a consistent set of initial conditions, and the second step is to compute the solution trajectory through integration. However, the algebraic constraints in the DAEs require initial conditions to be consistent with the differential equations, which may be quite difficult to be satisfied in the initialization phase. If the initial conditions are rather inaccurate and/or the system is highly nonlinear, iteration of the Newton-like solvers at the first step may diverge, converge slowly (i.e. stiff), or converge to an undesired solution. For simulations of large and complex systems, the computation time is usually dominated by the duration of the initialization phase (Tummescheit and Eborn 2002), which may significantly limit the computational efficiency of real time simulations. This study is concerned about the consistent initialization of a centrifugal chiller which is considered quite complicated as concatenation of several components, i.e., the centrifugal compressor, condenser, expansion device, and evaporator.

Centrifugal chiller is an important class of equipment for the HVAC systems for commercial buildings. There has been significant amount of work done on steady state modeling for centrifugal chillers (Braun *et al* . 1987; Beyene, *et al.* 1994; Gordon *et al*. 1995; Browne and Bansal 1998; Swider 2003; Saththasivam and Ng 2008). Dynamic modeling for centrifugal chillers is critical for developing advanced control technology and fault detection and identification (FDI) scheme. Bendapudi (2004) presented a work on the dynamic modeling of water-cooled centrifugal chiller. The simulation results agree with the steady-state data very well. However, there appeared some problems with initialization. According to Bendapudi, the model fails to converge for certain combinations of initial conditions and entering water temperature change rates during the earlier (<150s) part of the start-up process. This can be overcome by gradually and linearly ramping the entering water temperature from the initial to the final value over the first 120 to 150 seconds. In addition, the time consumed by the initialization process was significant. For a

1000-second simulation case as shown in Figure 1, the initialization process (i.e. the numerical transient) takes up about 1/3 of the total simulation time. Therefore, it is necessary to improve the initialization process and computational efficiency of the chiller simulation.

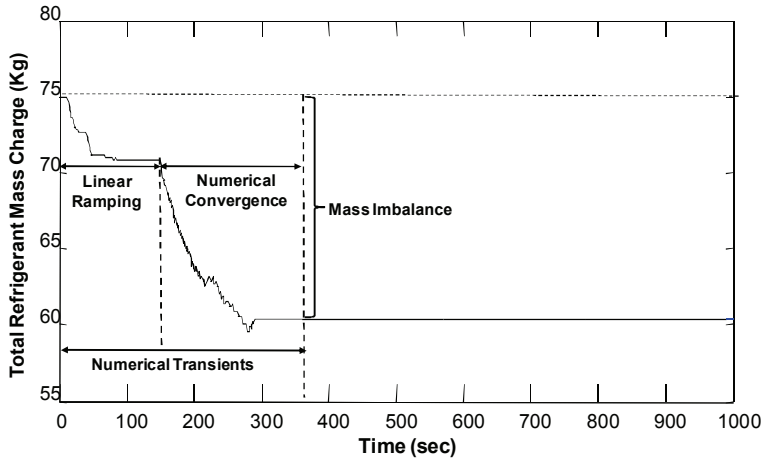


Figure 1: Total refrigerant mass charge at chiller start-up in fault-free condition, simulation of example 1 from Bendapudi (2004)

2. LITERATURE REVIEW ON DAE INITIALIZATION

The subject of consistent initialization of DAEs has been widely studied in the area of chemical engineering and applied mathematics. However, to the author's best knowledge, this topic has not been addressed in the domain of HVAC simulation and control. In general, there are two main kinds of methods for consistent initialization, i.e., the rigorous initialization techniques and the direct initialization methods (Kröner *et al.*, 1997). The rigorous initialization techniques typically require more knowledge from the structure of the DAE system. In addition, these methods generally require the solution of a set of non-linear algebraic equations.

Several rigorous initialization techniques have been studied in the literature. Probably the simplest method is the so-called *initial Euler step* methods. According to Sincovec *et al.* (1981), a DAE system with index v could be integrated with an implicit Euler method initially by dropping the error control. Consistent initial conditions will be reached at least v steps later. Then other desired integration methods with suitable error control should be switched on to further compute the solution trajectory. Albet *et al.* (1994) proposed a modified Euler step method to compute the derivatives of the variables after sudden changes in the operation conditions of the distillation columns. Two Euler steps were used to calculate the values of algebraic variables and their derivatives separately without any error control. According to Vieira and Biscaia (2001), the major drawback of the Euler step methods is that it makes no difference between variables that are already initialized and variables that must be determined. Considerable jumps will probably be observed in some of the state variables, and the user cannot control which variables are to be held constant. Hence, physical consistency of the initial conditions must be checked, as this method may result in impossible, or at least not desirable, initial conditions. The consistency equations methods are another class of rigorous initialization methods. Such methods typically require differentiation of the complete or part of the original DAE system, together with some user-specified information about the initial conditions, to formulate an extended set of DAEs which are called "consistency equations". The major limitation of this class of methods lies in that sometimes the numerical solution to the consistency equations may not converge, or even do not exist. Such difficulty arises from the fact that numerical solvers generally do not know which of the variables are determined by the constraints or the derivatives of the constraints and which are arbitrary.

The second class of methods work directly on the DAEs, thus known as the *direct initialization methods*. Such methods are simple and efficient with less dependence on the knowledge of the numerical solvers involved. Cuillé and Reklaitis (1986) worked on the modeling and simulation of staged batch distillation unit with chemical reactions in the liquid phase. A physically interpretable relaxation procedure was formulated to determine the consistent initial conditions. The discontinuity of the time derivatives of the solution at the starting point was approximated with a cubic polynomial transition function. An ad-hoc method proposed for steady-state initialization of some variables,

i.e., setting the time derivatives of some variables to zero, could not guarantee to work for all cases. The authors also mentioned that the initial time derivatives are generally non-zero in some physical processes. Kröner *et al.* (1997) presented a detailed analysis of the feasibility and applications of the direct initialization method. The authors limited the claim from other authors that steady state is always the consistent condition to semi-explicit index-1 DAE systems. Vieira and Biscaia (2001) proposed a direct initialization method based on the assumption that the dynamic response of a mathematical model may be approximated by the response to discontinuous perturbations of a similar system. Such a system should be in steady state before applying the perturbation. The proposed method has been tested with three classical benchmark models for the initialization process in chemical engineering area.

3. DIRECT METHOD FOR DYNAMIC CENTRIFUGAL COMPRESSOR INITIALIZATION

3.1 Problem Statement

The modeling details about the dynamic chiller model are described in Li *et al.* (2010a). The following will focus on the DAE initialization issue for the dynamic chiller model. The chiller components such as centrifugal compressor, condenser, evaporator, and expansion valve have been tested individually with the assumed boundary conditions and the simulations work very well. However, when the four components were connected together, simulation failed to start due to initialization problem. Figure 7 shows the failure message from Dymola simulation log.

```
ERROR: Failed to solve non-linear system using Newton solver.
To get more information: Turn on Simulation/Setup/Debug/Nonlinear
solver diagnostics/Details
Solution to systems of equations not found at time = 0
  Nonlinear system of equations number = 12
  Infinity-norm of residue = 1.10532E+006
  Iteration is not making good progress.
  Accumulated number of residue calculations: 90
  Last values of solution vector:
compressor.dischargeRefrigerant.h = 265504
compressor.portA.m_flow = 21.8338
  Last values of residual vector:
{ 32409.6, 1.07291E+006 }
```

Figure 7: Dymola simulation log of a failed initialization when the four chiller components are connected

The major problem is that the mass flow rates for the components should be solved implicitly based on the equations from each individual component. The transient mass balances at the condenser and evaporator reinforce the connection of the mass flow rates at each divided volume with thermal variables, which in turn affect the convergence of energy balance equations and/or constraints. For such a DAE system, consistent constraints should be satisfied in order for the numerical solver to compute its first integration step.

To solve such a problem in a systematic manner, the following remedies are proposed. For the initialization of the centrifugal compressor, a direct initialization method is proposed with three major steps. First, a reasonable compressor start-up speed command is computed from the knowledge of the compressor characteristic equation. Then, a pseudo physical analogy is established to approximate the initial mass flow rate solution from the centrifugal compressor. Second, a suitable perturbation function is applied to approximate the step function in order to perturb the compressor mass flow rate to its analytical non-surge solution. Finally, a variable modeling structure is proposed to switch the model equation back to the nonlinear compressor characteristic equation that includes surge solution. The details of each step of the direct initialization method are given later.

Besides the direct initialization method applied to the compressor mass flow rate solution, the initial conditions for the thermal variables at various states in the chiller cycle remain to be determined. To achieve this, a preprocessing scheme with another three steps is proposed. First, the initial guesses for the compressor discharge state are obtained based on the chiller design specification. Second, the initial conditions for the condenser are determined based on the inequality constraint established from the analysis of transient mass balance. Finally, the initial conditions for the evaporator are determined based on the inequality constraint established from the analysis of its minimum required

initial mass inventory associated with the transient change of mass storage in the condenser. The details of each step of the preprocessing scheme are described in Li *et al*. (2010b)

3.2 Compute Reasonable Compressor Start-Up Speed Command

For the refrigeration cycle of centrifugal chiller, the inlet refrigerant to the centrifugal chiller is typically saturated vapor, which could be analyzed based on the ideal gas law. According to Gravdahl (2002), the compressor characteristic could be expressed as

$$\psi_c\left(\omega,\dot{m}\right)=\left[1+\frac{\mu r_2^2\omega^2-\frac{r_1^2}{2}(\omega-\alpha\dot{m})^2-k_f\dot{m}^2}{c_pT_1}\right]^{\frac{\kappa}{\kappa-1}} \tag{1a}$$

$$\alpha\triangleq\frac{\cot\beta_{1b}}{\rho_1A_1r_1} \tag{1b}$$

where ψ_c is the pressure rise ratio, ω is the rotation speed of the drive motor, m is the mass flow rate. Unlike the air compression system in Gravdahl (2002), α is not a constant in chiller system, rather, it is a function of the inlet refrigerant density, which depends on the operation of chiller control at the evaporator side. β_{1b} is the refrigerant outflow angle at inducer, A_1 is the cross section area, r_1 is the average inducer radius. Also,

$$\mu\triangleq\sigma\left(1-\frac{\cot\beta_{2b}}{\rho_1A_1r_1}\frac{\dot{m}}{\omega}\right) \tag{1c}$$

where β_{2b} is blade angle at impeller tip, r_2 is the radius at impeller tip, k_f is the friction coefficient, T_1 is the inlet stagnation temperature, c_p is the specific heat capacity at constant pressure, κ is the heat capacity ratio and σ is the slip factor. Note that Equation 1(a) is valid for the whole range of compressor operation including the surge area. It can be analytically rearranged into

$$(k_f+\frac{1}{2}r_1^2\alpha^2)\dot{m}^2-r_1^2\omega\alpha\dot{m}+\frac{1}{2}r_1^2\omega^2-\mu r_2^2\omega^2+\psi_o=0 \tag{2a}$$

where

$$\psi_o\triangleq\left[\psi_c\left(\omega,\dot{m}\right)^{\frac{\kappa-1}{\kappa}}-1\right]c_pT_1 \tag{2b}$$

In Eq. 2(a), a nonlinear equation should be solved for the mass flow rate m. Fortunately, Eq. 2(a) is a quadratic equation which can be solved analytically. To get real solutions, the discriminant (Δ) of the quadratic equation should be greater than or equal to zero. In Eq. 2(a), Δ is given by,

$$\Delta=\left[(r_1^2\alpha)^2-4\left(k_f+\frac{1}{2}r_1^2\alpha^2\right)\left(\frac{1}{2}r_1^2-\mu r_2^2\right)\right]\omega^2-4\psi_0\left(k_f+\frac{1}{2}r_1^2\alpha^2\right) \tag{2c}$$

Solve for $\Delta\geq 0$, the constrain that should be satisfied is

$$\omega\geq\left[\frac{4\psi_0\left(k_f+\frac{1}{2}r_1^2\alpha^2\right)}{(r_1^2\alpha)^2-4\left(k_f+\frac{1}{2}r_1^2\alpha^2\right)\left(\frac{1}{2}r_1^2-\mu r_2^2\right)}\right]^{\frac{1}{2}} \tag{2d}$$

It is interesting to note that the solution of the mass flow rate is determined by the sign of Δ. If $\Delta<0$, there are one positive and one negative flow rate solutions. It can be easily seen that the negative solution should be neglected in the initialization period. On the other hand, if $\Delta>0$, then there are two positive solutions with a bigger one and a smaller one. A special case corresponds to when $\Delta=0$, the two solutions are identical with positive sign. For a given speed ω, the surge mass flow rate could be explicitly calculated based on Eq. 2(a). By taking the first derivative of ψ_c with respective to m and set it to zero, the surge point could be determined. By comparing the two possible

solutions with the surge point, the unstable solution could be detected and neglected. A closer look at Equation 2(c) reveals that the sign of Δ is also related to the rotation speed ω.

1) Mass flow rate $\dot{m}$ has one positive and one negative solutions for

$$\left[\frac{4\psi_0\left(k_f+\frac{1}{2}r_1^2\alpha^2\right)}{(r_1^2\alpha)^2-4\left(k_f+\frac{1}{2}r_1^2\alpha^2\right)\left(\frac{1}{2}r_1^2-\mu r_2^2\right)}\right]^{\frac{1}{2}}<\omega\le\left(\frac{\psi_0}{\frac{1}{2}r_1^2-\mu r_2^2}\right)^{\frac{1}{2}} \tag{3a}$$

2) Mass flow rate $\dot{m}$ has two positive solutions for

$$\omega>\left(\frac{\psi_0}{\frac{1}{2}r_1^2-\mu r_2^2}\right)^{\frac{1}{2}} \tag{3b}$$

3) Mass flow rate $\dot{m}$ has two identical positive solutions for

$$\omega=\left[\frac{4\psi_0\left(k_f+\frac{1}{2}r_1^2\alpha^2\right)}{(r_1^2\alpha)^2-4\left(k_f+\frac{1}{2}r_1^2\alpha^2\right)\left(\frac{1}{2}r_1^2-\mu r_2^2\right)}\right]^{\frac{1}{2}} \tag{3c}$$

The above constraints for ω provide a useful guideline to set the initial speed command. In addition, it provides a reasonable physical bound for the iteration range of ω, if the initial value of ω is determined by solving for other initial equations, e.g., the momentum balance equation that relates the drive torque τ_d, the compressor torque τ_c, and the rotation speed ω.

3.3 Formulate Pseudo-Physical Analogy for Centrifugal Compressor

One of the difficulties in centrifugal chiller initialization is to find consistent solutions of the valve flow rate and the compressor mass flow rate by simultaneously solving the nonlinear equations. It is then desirable to change the equation structure at the initialization phase. After the initialization, a suitable smoothing and switching method should be applied to switch back to the original DAE system. Compared to some rigorous initialization methods, the above scheme has more benefits in the following sense. In practice, a large jump reference can be avoided with an appropriate start-up controller. However, for simulation purpose, it is desirable to demonstrate such extreme behaviour as much as possible. Mathematically speaking, a jump start-up command corresponds to a step forcing function applied to the system. Physically, the change of mass flow rates and pressures from zero to finite values require a transient time period. However, in practice, the system behaviours in this transient time period are very difficult to measure. Therefore, it is very hard to predict the initial conditions, e.g., the initial derivatives of some state variables. Also, there is no general equations are strictly accurate in that short period. A remedy is to approximate the model behaviour in that period based on a suitable physical analogy[1]. It is important to note that such method is also very useful for other types of systems, for example, a sudden open/close of a valve, or a sudden command for the controller. The simplest pseudo-physical analogy would be a constant value, i.e.,

$$\dot{m}_0 = C \tag{4a}$$

where $\dot{m}_0$ is the initial mass flow rate and C is an arbitrary constant. Such method has been successfully applied to the calculation of correlations of heat transfer and pressure drop in TIL (Kossel *et al*. 2009). For a robust initialization, the correlations for heat transfer and pressure drop are switched from constant values to their actual correlations at different time instances during the simulation. For chiller simulation, an alternative form of the pseudo-physical analogy could be formulated since the pressure rise ratio and mass flow rate are coupled for the

[1] That is why it is termed as "pseudo-physical analogy".

initialization problem. Fortunately, we could use the compressor characteristic map to obtain a good start-up relation in the following form:

$$\dot{m}_0 = k_{initial}\psi_0 \tag{4b}$$

where $k_{initial}$ is a constant gain and ψ_0 is the initial pressure rise ratio. It is important to note that such a simple form is crucial for the success of the initialization problem. It is much easier for the numerical solver to treat this linear relation rather than the original nonlinear equation. Reducing the dimension of nonlinear system of equations could greatly facilitate the process of computing or approximating the inverse of Jacobian of the DAE system by Newton-like solvers.

3.4 Perturbation Method

After the pseudo-physical analogy is established, the step function is approximated with the following perturbation function

$$\dot{m}(t) = \left[1 - \delta(t - t_c, \Delta t)\right]\dot{m}_0 + \delta(t - t_c, \Delta t)\dot{m}_1 \tag{5}$$

where $0 \le \delta(t - t_c, \Delta t) \le 1$, with t being the current simulation time, t the transition time to apply the step change, and Δt the time to complete the perturbation. The selection of an appropriate perturbation function $\delta(t - t_c, \Delta t)$ is given in later section with details. $\dot{m}_0$ is the mass flow rate obtained from the pseudo-physical analogy shown in Equation 4. The selection of $\dot{m}_1$ could be facilitated by examining the compressor characteristic map. Depending on the rotation speed ω, the solutions from Equation 2(a) could be one negative and one positive or two positive solutions, however, in either case, the solution on the right-hand side of the surge point can be uniquely determined by a single expression, i.e.,

$$\dot{m}_1 = \frac{r_1^2\alpha\omega + \sqrt{(r_1^2\alpha\omega)^2 - 4\left(k_f + \frac{1}{2}r_1^2\alpha^2\right)\phi}}{2\left(k_f + \frac{1}{2}r_1^2\alpha^2\right)} \tag{6}$$

3.5 Variable Structure Modeling and Reinitialization

The perturbation method described in the previous section tunes the mass flow rate solution to a stable one. However, for centrifugal chillers, it is often desirable to simulate unstable (but realistic) behavior like surge and stall for the study of dynamics and control. For such purpose, it is necessary to switch back to the nonlinear equations in the centrifugal compressor model. It is important to note that such a switch involves two crucial issues in the area of numerical simulation, i.e., variable structure modelling and consistent initialization for reinitialization after the discontinuity jump introduced by switching the models.

Model switching during simulation dynamically changes the effective DAE system. At the switching time, the numerical solver has to stop and a new set of consistent initial conditions should be obtained in order for the solver to continue. In Dymola, switching from model $f_1(\bullet)$ to model $f_2(\bullet)$ during simulation can be realized by:

$$0 = \left(1 - \lambda(t)\right) f_1(\dot{m}_1) + \lambda(t) f_2(\dot{m}_2) \tag{7a}$$

where

$$f_1(\dot{m}_1) = \dot{m}_1 - \frac{r_1^2\alpha\omega + \sqrt{(r_1^2\alpha\omega)^2 - 4\left(k_f + \frac{1}{2}r_1^2\alpha^2\right)\phi}}{2\left(k_f + \frac{1}{2}r_1^2\alpha^2\right)}, \tag{7b}$$

$$f_2(\dot{m}_2) = (k_f + \frac{1}{2}r_1^2\alpha^2)\dot{m}_2^2 - r_1^2\omega\alpha\dot{m}_2 + \frac{1}{2}r_1^2\omega^2 - \mu r_2^2\omega^2 + \psi_o, \tag{7c}$$

and

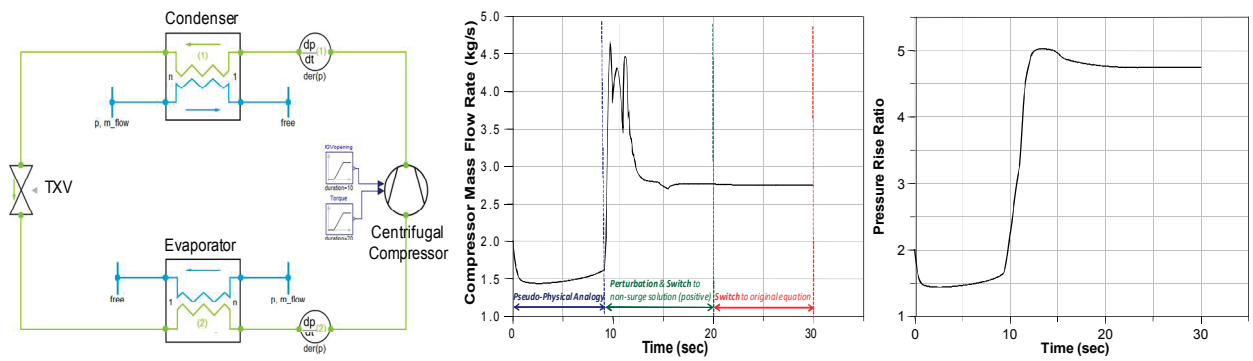
$$\lambda(t) = \begin{cases} 0 & t < t_s \\ 1 & t \ge t_s \end{cases}. \tag{7d}$$

where t is the current simulation time and t_s is the time instant for model switching.

4. SIMULATION STUDY

4.1 Simulation Results of the Direct Initialization Method

Simulation study was conducted to evaluate the developed dynamic model for the centrifugal chiller with the proposed initialization method, with R134a as the refrigerant. The inlet water flow rates of the condenser and evaporator were 16.7kg/s and 13.2kg/s, respectively. The inlet water temperatures of the condenser and evaporator were 22°C and 16°C, respectively. Figure 2(a) shows the Dymola layout of the centrifugal chiller model. Figure 2(b) shows the compressor mass flow rate during the initialization period (0 ~ 30 seconds). Note that as shown in Figure 2(b), the second transition (9 ~ 20 seconds) is necessary for the Newton iteration solver to converge for the next transition (20 ~ 30 seconds). The corresponding solution profile of the pressure rise at the centrifugal compressor is given in Figure 2(c).

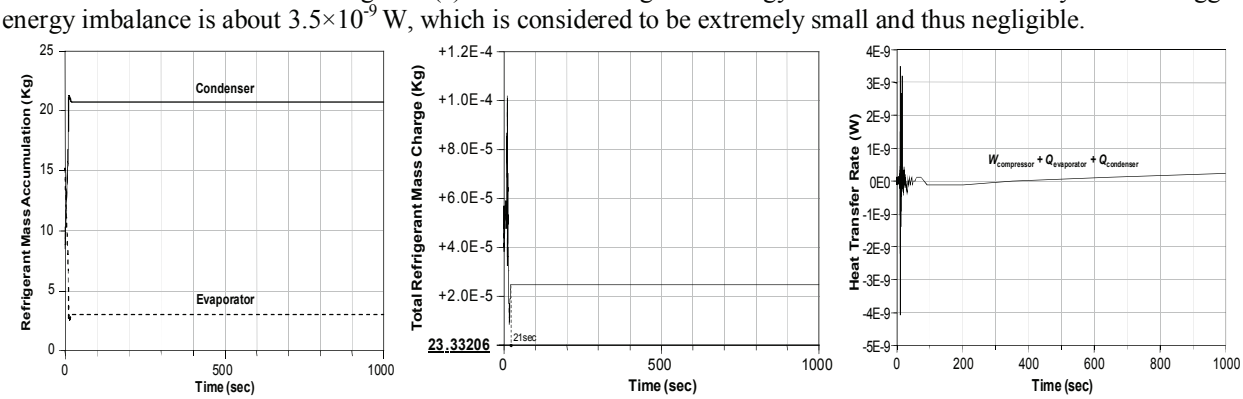


(a) (b) (c)

Figure 2: Simulation study of the proposed initialization method where (a) is the Dymola layout of the centrifugal chiller model, (b) is the mass flow rate at compressor outlet during the initialization phase and (c) is the pressure rise ratio during the initialization phase

4.2 Check of Conservation of Mass and Energy

Due to perturbation method used in this study, it is important to check the mass and energy conservation during the initialization phase and the steady-state. Figure 3(a) shows the mass accumulations at the condenser and evaporator, respectively, and Figure 3(a) shows the solution profile for the total refrigerant mass charge. As can be observed in Figure 3(a), the amount of mass imbalance is only detectable by the end of the perturbation method, i.e., 21 seconds. However, this amount of mass imbalance is extremely small within about 0.0004% of the total refrigerant mass and is thus considered to be negligible. For the check of refrigerant energy balance in the chiller cycle, at any simulation time, the work input to the centrifugal compressor plus the heat transferred to the evaporator should equal to the heat removed from the condenser. Figure 3(c) shows the refrigerant energy balance in the chiller cycle. The biggest energy imbalance is about 3.5×10^{-9} W, which is considered to be extremely small and thus negligible.



(a) (b) (c)

Figure 3: (a) is the refrigerant movement during start-up and steady state mass accumulation in the condenser and evaporator, respectively, (b) is the total refrigerant mass charge in the chiller cycle (check of mass conservation) and (c) is the total refrigerant energy balance in the chiller cycle (check of energy conservation)

6. CONCLUSIONS

In this paper, the dynamic model of a water-cooled centrifugal chiller is developed based on Modelica. A preprocessing scheme was proposed to deal with the chiller initialization problem. First, the reasonable initial values for the chiller system simulation are computed once the geometric parameters and design conditions are available. Then, a direction method was proposed for the consistent initialization of dynamic centrifugal chiller system. The direction method consists of three major steps: 1) establish a pseudo-physical analogy, 2) apply the perturbation method, and 3) switch the model structure. Simulation results have demonstrated the effectiveness of proposed initialization method.

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