Modeling Adjustable Throat-Area Expansion Valves

Haorong Li
Purdue University

James E. Braun
Purdue University

Bo Shen
Purdue University

Modeling Adjustable Throat-Area Expansion Valves

Haorong Li, James E. Braun, and Bo Shen

Purdue University, School of Mechanical Engineering
Ray W. Herrick Laboratories
West Lafayette, IN 47906, USA
Phone: (765)-496-7515; Fax: (765)-494-0787; Email: lihaoron@ecn.purdue.edu

ABSTRACT

Adjustable throat-area expansion valves (ATAEV), including thermostatic and electric expansion valves, are used commonly in air conditioning equipment and lead to improved system performance as compared with the use of fixed orifice expansion devices. However, ATAEV modeling literature is limited. Typically, a TXV is modeled by specifying the superheat entering the compressor or empirically correlating experimental data. In order to model system behavior more accurately and effectively over a wide range of conditions, more accurate ATAEV models are necessary and a more general modeling methodology is desired. The current paper presents a general model format that utilizes manufacturers' rating data. Model structures for three types of valve geometries are derived. Two model formats and parameter estimation procedures using manufacturer performance rating data were considered. The proposed methods are validated using experimental data and compared with results in the literature. Both experimental validation and theoretical analysis demonstrate that the proposed methods are more accurate and more generic than other methods presented in the literature.

1. INTRODUCTION

Expansion devices reduce the pressure and regulate the refrigerant flow to the low side evaporator within a vapor compression system. A model of the expansion device is essential to simulate the whole system and can be used as a virtual sensor to estimate its upstream pressure as part of an automated diagnostic system (see Li and Braun (2004)).

There are two kinds of expansion devices used in vapor compression systems: fixed-area and adjustable throat-area devices. The drawback associated with fixed-area devices is their limited ability to efficiently regulate refrigerant flow in response to changes in system operating conditions, since they are sized based on one set of conditions. Adjustable throat-area expansion valves provide a better solution to regulating refrigerant flow into a direct expansion type evaporator using certain feedback control strategy. A thermostatic expansion valve (TXV) and an electric expansion valve (EXV) are two types of adjustable throat-area expansion valves. A TXV is a completely mechanical device that uses a single variable proportional feedback control scheme to maintain a nearly constant superheat at the evaporator outlet. The fundamental principle of an EXV is the same as a TXV except that it uses electronic actuation and sensor information along with a digital feedback controller and can theoretically operate with a smaller degree of superheat than a TXV. There is a lot of literature for modeling and experimental investigations for fixed orifice devices. Although TXVs and EXVs are used widely, there is very little literature related to modeling of their behavior. In some simulation models for unitary heat pumps such as PUREZ (Rice, 2001), models for TXVs and EXVs are simplified by explicitly fixing a constant superheat or implicitly specifying superheat trends. Browne and Bansal (1998) described a modeling method using the difference of the superheat in the evaporator to the reference superheat temperature to modify the fixed orifice model. Harms (2002) showed that constant superheat was a poor assumption and correlated TXV performance using experimental data. Among the limited literature, none discusses fundamentally whether the flow is choked or not. In the limited literature, the following format for a TXV model has been generally adopted,

$$\dot{m} = CA\sqrt{r(P_{up} - P_{down})} \quad (1)$$

where, C is discharge coefficient, A is the throat area, r is density, P_{up} is the upstream pressure, P_{down} is the downstream pressure. The above equation is the same as that for an orifice except that A is a variable. Therefore, it seems that mass flow rate is a strong function of pressure drop $DP = P_{up} - P_{down}$ and variable restriction area A, but a very weak function of upstream refrigerant subcooling, T_{sub}. The implicit assumption is that the flow is not choked. Benjamin and Miller (1941) conducted experiments of sharp-edged orifices of $L/D = 0.28 \sim 1$ with saturated water at various upstream pressures and found that orifices having $L/D < 1$ did not choke the flow at normal operating conditions. However, some researchers (Chisholm, 1967; Krakow and Lin 1988) observed that the mass flow rate of a refrigerant through an orifice in a heat pump was primarily dependent on the upstream conditions, which indicates that the flow was choked. This warrants further investigation. Before using this model format, it is advisable to validate this assumption.

2. Approach

In this section, the general model format is validated using manufacturers' data, mathematical expressions are derived that relate throttle area to valve position and valve position to superheat, and procedures are presented for estimating model parameters from manufacturers' rating data.

2.1 Model Format Validation Using Manufacturers' Rating Data

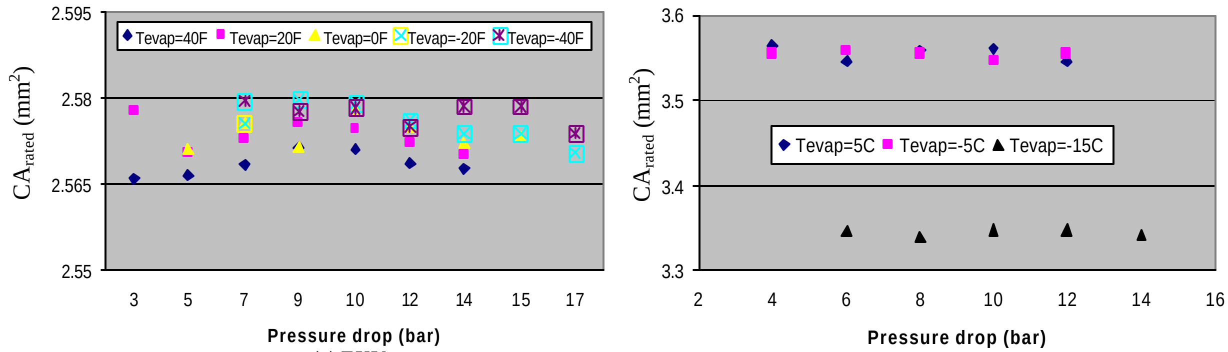
Whether the flow is choked or not can be checked indirectly by analyzing manufacturers' rating data. Equation (2) can be rearranged as,

$$CA = \frac{\dot{m}_{ref}}{\sqrt{r\,(P_{up} - P_{down})}} \tag{2}$$

According to ANSI/ASHRAE standard 17 (1998) and ARI standard 750 (2001), throat-area A is nearly fixed by fixing the opening superheat when generating the manufacturers' rating data for a TXV. For an EXV, the throat-area A is exactly fixed at the rating value. So CA_{rated} for an EXV should be constant and that for a TXV should be relatively constant if the flow is not choked.

Figure 1a shows that CA_{rated} for a 3.5-ton EXV is pretty constant (mean: 2.5736 mm^2, standard variation: 0.0038 mm^2) over the whole set of rating conditions (evaporator temperature: -40F~40F and Pressure Drop: 50psi~250psi). For a 5-ton TXV, Figure 1b shows that CA_{rated} has an abrupt change from an air conditioning application (evaporator temperature: -5C ~ 5C) to a refrigeration application (evaporator temperature: -15C). In spite of the abrupt change, its overall variation is still small (mean: 3.4842 mm^2, standard variation: 0.1020 mm^2). However, the variation is very small within each application range. For air conditioning applications, the mean is 3.5538 mm^2, and standard variation is 0.0068 mm^2. For refrigeration applications, the mean is 3.3451 mm^2, and standard variation is 0.0041 mm^2. Therefore, the TXV model format is accurate at the rating conditions and the flow is not chocked.

The abrupt change in CA_{rated} for the TXV can be explained by the saturation pressure-temperature (P-T) curve for the thermostatic charge fluid. Figure 2 shows that the P-T curve becomes flatter at lower temperature. As a result, a given opening superheat results in less pressure difference across the valve diaphragm at lower evaporating temperatures causing a reduction in valve opening area. For example, the pressure difference caused by 5 C of opening superheat at an evaporating temperature of 5 C is 0.969 bars, which is far larger than 0.584 bars at an evaporating temperature of -15 C. Fortunately, this would not cause any problem in modeling because 1) the P-T curve is pretty linear if it is divided into three sections: AB, BC and CD; 2) for a given application, the TXV will work in one of the three sections and the TXV used in packaged air conditioning falls into section CD; 3) the nonlinearity can be eliminated or overcome using cross charges. For cross charges, the TXV working fluid is chosen so that the opening force is nearly proportional to opening superheat over the entire operating range.



(a) EXV (b) TXV

Figure 1 The CA_{rated} values of an EXV and a TXV under manufactory ratings

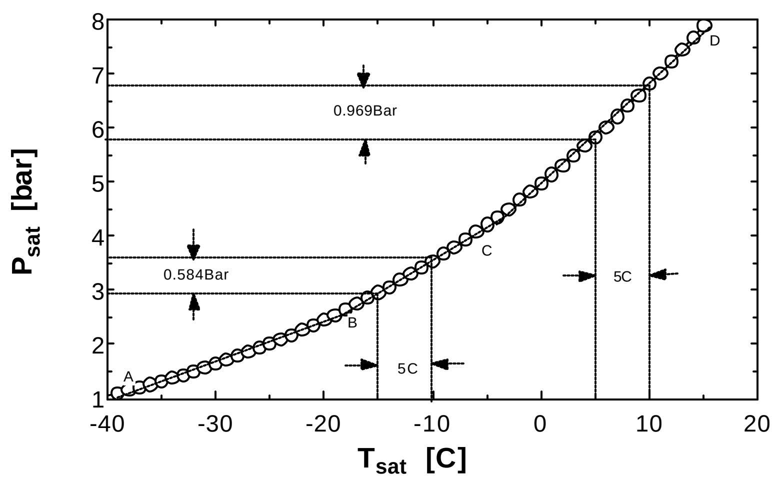


Figure 2 P-T saturation curve for R22

In summary, from manufacturers' standard rating data, the flow across a TXV or EXV is not choked and the generally used model format is valid. To specify a TXV or EXV model, the key point is to find an expression for variable throat-area, A, in terms of superheat and then specify the constant C using manufacturers' rating data. Generally speaking, the throat-area, A, is a function of valve position, which is determined by the control strategy used by the valve. Because TXVs and EXVs use different control strategies, the first step is to derive the A in terms of valve position and then develop expressions for valve position in terms of superheat.

2.2 Derivation of Throat-Area, A, Expression

As shown in Figure 3, there are three kinds of valves used in TXVs and EXVs. Among them, types I and II are used widely and their geometric model is the same.

Figures 4a and 4b illustrate TXV valves at an operating point. At a certain valve position, h, the throat-area is,

$$A = \frac{\pi}{4}(D^2 - d^2),$$

where $d = 2\tan\theta\,(H-h)$ and $\tan\theta = \dfrac{D}{2H}$, so,

$$d = 2\frac{D}{2H}(H-h) = D(1-\frac{h}{H}),$$

These equations can be combined to give,

$$A=\frac{p}{4}(D^2-D^2(1-\frac{2h}{H}+(\frac{h}{H})^2))=\frac{p}{2}D^2(\frac{h}{H}-\frac{1}{2}(\frac{h}{H})^2)=\frac{p}{4}\frac{h}{H}D^2(2-\frac{h}{H})$$

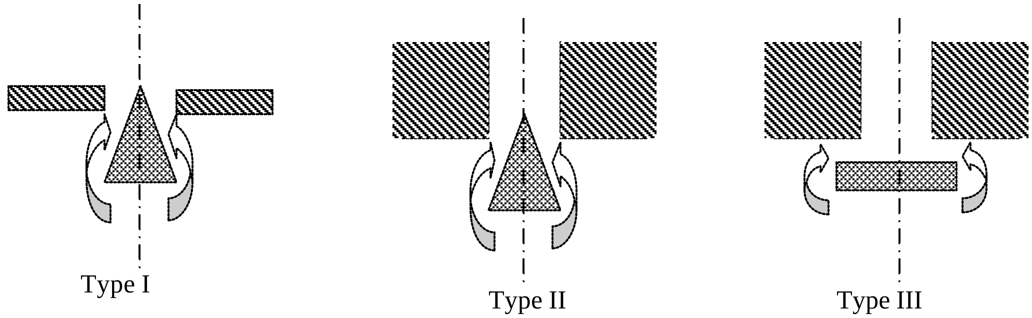


Figure 3 Three types of valve geometry

It is obvious that throat-area, A, is a second order function of valve position, h, which is plotted as Figure 4c. Figure 4b shows the geometric model for valve type III. An expression for throat area in terms of valve position is

$$A = pDh\ ,$$

It can be seen that the throat-area, A, is a linear function of valve position, h. It is plotted in Figure 4c

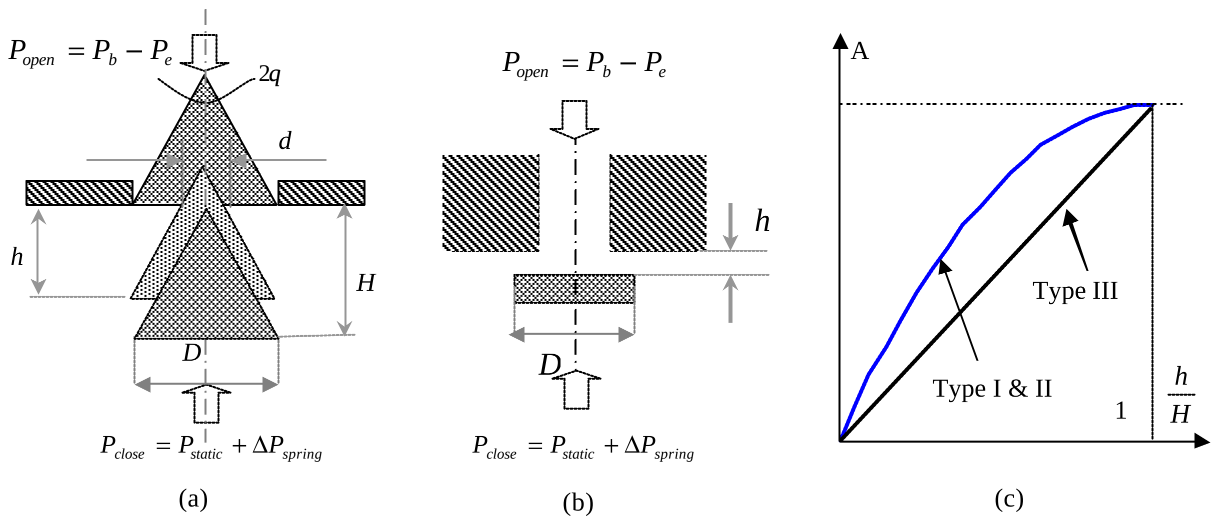


Figure 4 Geometric models and throat-area curves for different valve types

2.3 Valve Position Expression

The valve position for an EXV can be calculated easily from the control signal,

$$h = f(control\_signal)\ .$$

where $control\_signal$ is determined by the control algorithm and can be a function of various thermodynamic parameters.

For a TXV, valve position is a function of superheat. As shown in Figures 4a and 4b, the pressure of the thermostatic element, P_b, is applied to the top of the diaphragm and acts to open the valve; the evaporator temperature, P_e, is applied under the diaphragm and acts in a closing direction; P_{static} is caused by the initial spring deformation which is preset by initial static superheat setting and acts to close the valve; DP_{spring} is the pressure caused by extra spring deformation other than the initial static superheat setting and acts to close the valve. So, the pressure difference between P_b and P_e acts to open the valve. Assume that the P-T curve is linear in the range of operation, and then the pressure difference across the diaphragm (P_{open}) is a linear function of opening superheat, $T_{sh,opening}$,

$$P_{open} = P_b - P_e = k_1 T_{sh,operating} \,,$$

and according to Hooke's Law, the total spring force, P_{close}, is proportional to the total spring deformation,

$$P_{close} = P_{static} + DP_{spring} = k_2 (x_{static} + h) \,.$$

At any constant operating condition, the forces exerted on the valve are balanced,

$$k_1 T_{sh,operating} = k_2 (x_{static} + h) \,,$$

Rearranging the above equation gives an expression for valve position,

$$h = \frac{k_1}{k_2} T_{sh,operating} - x_{static} = kT_{sh,operating} - x_{static} = kT_{sh,operating} - kT_{sh,static} = k(T_{sh,operating} - T_{sh,static}) = kT_{sh,opening} .$$

As shown in Figure 5a, the valve position is a linear function of opening superheat.

2.4 Overall Mass Flow Rate Model for a TXV

For an EXV, the overall mass flow rate model can be obtained by substituting the throat-area into Equation (1) and coupling the valve position to a specific feedback controller algorithm.

The overall mass flow rate model for a TXV can be obtained by substituting the expressions for throat-area and valve position into the general model equation.

For type I and II valves, this leads to

$$\begin{aligned} A &= \frac{pD^2}{4}\frac{h}{H}(2 - \frac{h}{H}) = \frac{pD^2}{4}\frac{kT_{sh,opening}}{H}(2 - \frac{kT_{sh,opening}}{H}) \\ &= \frac{pD^2}{4}\frac{kT_{sh,\max opening}}{kT_{sh,\max opening}}(2 - \frac{kT_{sh,opening}}{kT_{sh,\max opening}}) = \frac{pD^2}{4}\frac{T_{sh,opening}}{T_{sh,\max opening}}(2 - \frac{T_{sh,opening}}{T_{sh,\max opening}}) \end{aligned}$$

$$\begin{aligned} \dot{m} &= C_d A \sqrt{r(P_{up} - P_{down})} = C_d \frac{pD^2}{4}\frac{T_{sh,opening}}{T_{sh,\max opening}}(2 - \frac{T_{sh,opening}}{T_{sh,\max opening}})\sqrt{r(P_{up} - P_{down})} \\ &= C(2\frac{T_{sh,opening}}{T_{sh,\max opening}} - (\frac{T_{sh,opening}}{T_{sh,\max opening}})^2)\sqrt{r(P_{up} - P_{down})} \end{aligned}$$

For type III valves,

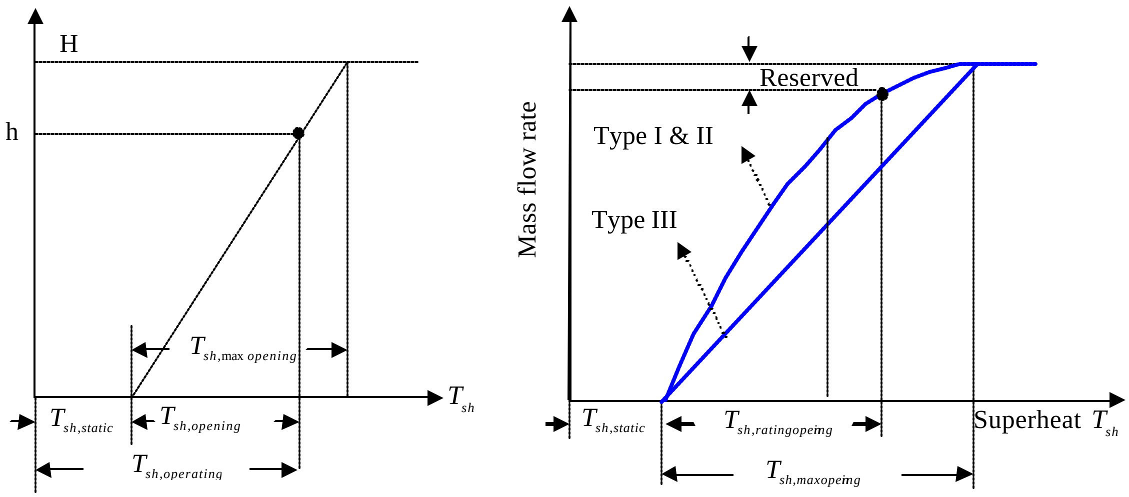
$$A = pDkT_{sh,opening}$$

$$\begin{aligned} \dot{m} &= C_d A \sqrt{r(P_{up} - P_{down})} = C_d pDkT_{sh,opening}\sqrt{r(P_{up} - P_{down})} \\ &= CT_{sh,opening}\sqrt{r(P_{up} - P_{down})} \end{aligned}$$

Figure 5b shows refrigerant mass flow rate versus superheat for a fixed pressure drop. It can be seen that:

1) The mass flow rate for type I & II valves is higher than that for type III valves with the same operating range and at the same superheat, except when the valves are fully open or close. Therefore, for valves with the same operating range, type I & II valves require smaller superheat to get the same capacity as type III valves.
2) The mass flow for type III valves increases linearly with superheat until the maximum opening superheat is reached, whereas for type I & II valves, mass flow rate increases nonlinearly and the rate of increase

approaches zero when the valve is fully open. When the valve is fully open, the mass flow is larger than that at the rated condition and so is the capacity. The additional capacity beyond the rated is termed reserve capacity. Since the increase rate of mass flow rate decreases, for type I & II valves to have the same reserve capacity as type III valves, more superheat is required. In other words, type I & II valves would be expected to have smaller reserve capacity (around 10%) than that of type III (up to 40%) valves in order to avoid abnormally high superheat at high capacity operation. However, an advantage of type I & II valves is a reduction in TXV cycling ("hunting") caused by the TXV alternately overfeeding and underfeeding the evaporator.



(a) Valve position curve (b) Valve mass flow rate curve at fixed pressure drop

Figure 5 Valve position and mass flow rate curves

2.5 Model Parameter Estimation

Since the overall mass flow rate model for EXVs is explicit, all the parameters are available. From the above analysis, it can be seen that the mass flow rate for type I and II TXVs is a nonlinear function of superheat while that of type III is a linear function of superheat. However, in most of the existing literature, it is assumed that the mass flow rate for all kinds of TXV is a linear function of superheat. So, in order to simplify the parameter estimation, a globally linear assumption can be adopted (no approximation for type III TXV). Alternatively, the nonlinear model can be employed with a more complicated method for estimating parameters with additional assumptions. Both approaches are considered in this section.

2.5.1 Globally Linear Model

Under the global linear assumption, the general TXV model is

$$\dot{m} = C(T_{sh,operating} - T_{sh,static})\sqrt{r(P_{up} - P_{down})}$$

Rearranging the above equation,

$$C(T_{sh,operating} - T_{sh,static}) = \frac{\dot{m}}{\sqrt{r(P_{up} - P_{down})}}$$

The parameters of this TXV model can be determined using the following procedure,

1) According to manufacturers' rating data,

$$C(T_{sh,rating} - T_{sh,static}) = CT_{sh,ratingopening} = CONSTANT \ ,$$

where $T_{sh,ratingopening}$ is fixed by the TXV manufacturer and should be readily available. Although the TXV manufacturer presets the $T_{sh,static}$ as well, the manufacturer of an air conditioning system would adjust it slightly in order to match the rated capacity.

2) IF $T_{sh,ratingopening}$ is available from the manufacturer, go to step 3. If not, roughly guess an initial value according to ARI and ASHRAE standards and manufacturing tradition (Table 1).

Table 1 TXV rating settings

Source	$T_{sh,rating,opening}$ (C)	$T_{sh,rating}$ (C)	$T_{sh,static}$ (C)	Reserve Capacity
ARI Standard	≤ 4		> 1	
ASHRAE Standard Example	3		3	
ASHRAE Handbook	2 ~ 4			0.1 ~ 0.4
ALCO (recommend)	2.2 ~ 3.3		3.3 ~ 5.6	
SPORLAN(recommend)		4.4 ~ 6.7		
Recommended Initial Guess	3 or 4		3, 4 or 5	0.1

3) Determine $C = \dfrac{CONSTANT}{T_{sh,ratingopening}}$.

4) Determine $T_{sh,static}$. If the number of rotations adjusted by the system manufacturer is recorded, it could be easy to calculate the actual static superheat. If not, it could be estimated from the manufacturer settings and refined by experimental data.

5) Determine $T_{sh,\max opening}$ using the manufacturers' tradition of reserving capacity ($reserve\_capacity$) to set the upper boundary of $(T_{sh,rating} - T_{sh,static})$.

$$\frac{T_{sh,ratingopening}}{T_{sh,\max opening}} \approx 1 - reserve\_capacity$$

2.5.2 Nonlinear Model

The nonlinear model format is

$$\dot{m} = C\left(2\frac{T_{sh,opening}}{T_{sh,\max\ opening}} - \left(\frac{T_{sh,opening}}{T_{sh,\max\ opening}}\right)^2\right)\sqrt{r(P_{up} - P_{down})}$$

Rearranging the above equation,

$$C\left(2\frac{T_{sh,opening}}{T_{sh,\max\ opening}} - \left(\frac{T_{sh,opening}}{T_{sh,\max\ opening}}\right)^2\right) = \frac{\dot{m}}{\sqrt{r(P_{up} - P_{down})}}$$

The parameters of the nonlinear TXV model can be determined using the following procedure,

1) According to manufacturers' rating data, $C\left(2\frac{T_{sh,ratingopening}}{T_{sh,\max\ opening}} - \left(\frac{T_{sh,ratingopening}}{T_{sh,\max\ opening}}\right)^2\right) = CONSTANT$

2) According to manufacturers' tradition of reserving capacity,

$$\left(2\frac{T_{sh,ratingopening}}{T_{sh,\max opening}} - \left(\frac{T_{sh,ratingopening}}{T_{sh,\max opening}}\right)^2\right) \approx 1 - reserve\_capacity$$

$$\Rightarrow C = \frac{CONSTANT}{1 - reserve\_capacity},$$

and solving the equation,

$$\frac{T_{sh,ratingopening}}{T_{sh,\max\ opening}} = 1 - \sqrt{reserve\_capacity}$$

3) Determine $T_{sh,static}$ and $T_{sh,ratingopening}$ as described in the last section,

4) Determine $T_{sh,\max,opening}$ and set the upper boundary for $(T_{sh,rating} - T_{sh,static})$.

3. Validation Using Laboratory Data

Data for a 5-ton RTU collected by Harms (2002) were used to validate the TXV Model.

3.1 Globally Linear Model

According to the manufacturers' rating data,

$$C(T_{sh,rating} - T_{sh,static}) = CONSTANT = 3.5576 \quad mm^2$$

From experimental data set A from Harms (2002) with a nominal charge, it can be estimated that

$$T_{sh,rating} = 8^\circ C$$

Assuming $T_{sh,ratingopening} = 4^\circ C$, so

$$T_{sh,static} = T_{sh,rating} - T_{sh,ratingopening} = 8 - 4 = 4^\circ C$$

and

$$C = \frac{3.5576}{4} = 0.8894$$

Assuming the reserve capacity is 10%, since most valves are type I & II,

$$T_{sh,\max,opening} \approx \frac{T_{sh,rating,opening}}{1 - reserve\_capacity} = \frac{4}{0.9} \approx 4.5$$

So,

$$\begin{aligned}\dot{m} &= C(T_{sh,operating} - T_{sh,static})\sqrt{r(P_{up} - P_{down})} \\ &= 0.8894\,(T_{sh,operating} - 4)\sqrt{r(P_{up} - P_{down})}\end{aligned}$$

where the upper boundary of $(T_{sh,rating} - T_{sh,static})$ is set at $4.5^\circ C$ and the unit for P_{up} and P_{down} is Pa.

3.2 Nonlinear Model

According to the manufacturers' rating data,

$$C\left(2\frac{T_{sh,ratingopening}}{T_{sh,\max\ opening}} - \left(\frac{T_{sh,ratingopening}}{T_{sh,\max\ opening}}\right)^2\right) = CONSTANT = 3.5576 \quad mm^2$$

Assuming reserve capacity of 10%,

$$C = \frac{CONSTANT}{1 - reserve\_capacity} = \frac{3.5576}{0.9} = 3.9529$$

and,

$$\frac{T_{sh,ratingopening}}{T_{sh,\max\ opening}} = 1 - \sqrt{reserve\_capacity} = 1 - \sqrt{0.1} = 0.68$$

Assuming $T_{sh,ratingopening} = 4^\circ C$,

$$T_{sh,\max\ opening} = \frac{4}{0.68} \approx 6^\circ C$$

So,

$$\dot{m} = C(2\frac{T_{sh,opening}}{T_{sh,\max opening}} - (\frac{T_{sh,opening}}{T_{sh,\max opening}})^2)\sqrt{r(P_{up}-P_{down})} = 3.9529(2\frac{T_{sh,opening}}{6} - (\frac{T_{sh,opening}}{6})^2)\sqrt{r(P_{up}-P_{down})}$$

where, the upper boundary of $(T_{sh,rating} - T_{sh,static}) = T_{sh,opening}$ is set at $6^\circ C$ and the unit for P_{up} and P_{down} is Pa.

3.3 Comparison with Laboratory and Model from Harms

Harms plotted all four sets of data (see Figure 6) and fit the following model by minimizing the least squares error.

$$\dot{m}_{ref} = c_1(T_{super} - c_2)[r_f(P_{up} - P_{down})]^{0.5}$$

Harms determined $c1 = 0.51\, mm^2/^\circ C$, $c2 = 1.0^\circ C$. So,

$$\dot{m} = 0.51(T_{sh,operating} - 1)\sqrt{r(P_{up} - P_{down})}$$

where the upper boundary of $(T_{sh,operating} - 1)$ was set at $8^\circ C$.

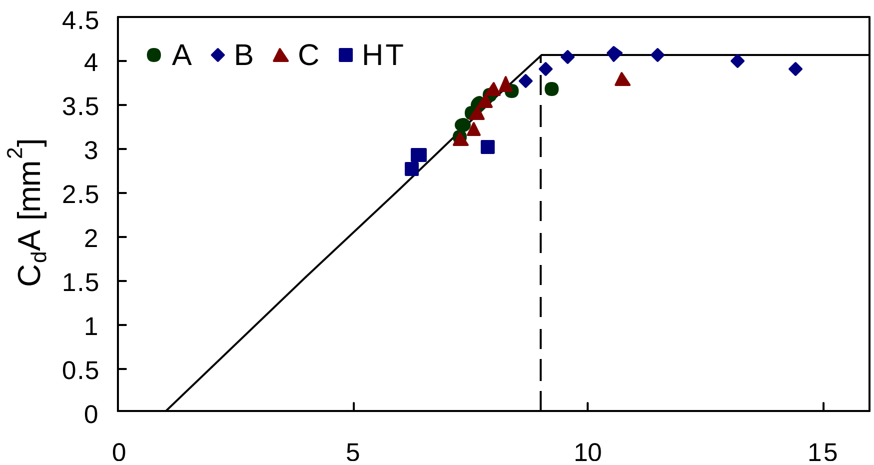


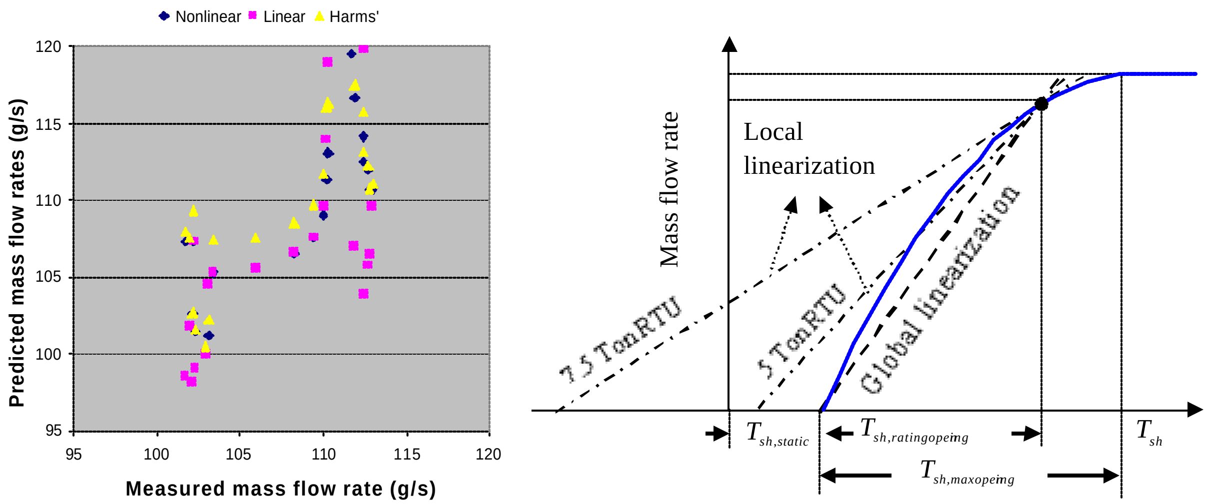
Figure 6 $C_d A$ value for a 5-ton RTU TXV as a function of superheat

Figure 7a and Table 2 show results for the globally linear and nonlinear modeling approaches along with results from a correlation model presented by Harms. The model developed by Harms used all of the data from Figure 7a to train the model. It is obvious that the nonlinear model provides better predictions than the globally linear model and comparable accuracy to the interpolation performance of Harms' model.

Although Harms' empirical mo del may be good for interpolation, it can not be expected to extrapolate well. Mathematically, this model is equivalent to making a locally linear assumption (see Figure 7b). If the experimental data range is limited, parameters C_1 and C_2 will be unreasonable. For example, the parameter C_2 from Harms for the 5-ton RTU, which is supposed to be the static superheat setting, is equal to $1^\circ C$, while the upper boundary of opening superheat is set at $8^\circ C$. According to ARI and ASHRAE standards, static superheat should be far larger than $1^\circ C$, and $8^\circ C$ for an upper boundary on opening superheat (indicating a 50% of reserve capacity) is too large. For a 7.5 ton RTU considered by Harms, parameter C_2 was correlated to be a negative value, $-4.4^\circ C$, which is impossible physically.

Table 2 Comparison of relative error for mass flow rate predications

	Nonlinear Model	Global Linear Model	Harms Results
Mean	0.0096	-0.0043	0.0235
Std.	0.0291	0.0460	0.0352
Spread	0.0967	0.1647	0.1329



(a) Comparison of three models' predictions (b) Illustration of three modeling methods

Figure 7 Comparison of the three modeling methods

4. Conclusions

The model format for adjustable-area expansion devices was validated using manufacturer's data and the flow through the adjustable-area expansion devices is not choked. Expressions for throat areas were derived as a function of valve position and superheat, which leads to the mass flow rate model. Two model formats and parameter estimation procedures were considered and their predictions were compared with laboratory measurements. The nonlinear modeling approach only requires data at a rating condition to obtain parameters and gave good predictions over a wide range of operating conditions when compared with laboratory data.

5. References

ARI, 2001, Standard 750, Thermostatic Refrigerant Expansion Valves, Air-conditioning & Refrigeration Institute, Arlington, VA.

ASHRAE, 1998, STANDARD 17, Method of Testing Capacity of Thermostatic Refrigerant Expansion Valves, American Society of Heating, Refrigerating and Air-conditioning Engineers, Atlanta, GA.

Benjamin, M.W., and J.G. Miller,1941. The flow of saturated water throttling orifice. Transactions of the ASME 63 (5): 419-426

Browne, W. Matthew and Bansal, K. Pradeep, 1998. Challenges in Modeling Vapor-Compression Liquid Chillers, AHRAE Trans., 1998, V. 104, Pt. 1.

Chisholm, D. 1967. Flow of compressible two-phase mixtures through throttling devices. Chemical and Process Engineering, vol. 48:342-350

Harms, Todd M., 2002. Charge Inventory System Modeling and Validation for Unitary Air Conditioners, Ph.D. Thesis, School of Mechanical Engineering, Purdue University.

Krakow, K.I., and Lin, S., 1988, Refrigerant flow through orifices, AHRAE Trans., 94(1):484-506

Li, H. and Braun, J.E., 2004a, "A Methodology for Diagnosing Multiple-Simultaneous Faults in Rooftop Air Conditioners" . Accepted for the Tenth International Refrigeration and Air Conditioning Conference at Purdue to be held on July 12-15, 2004.

Rice, C. Keith, 1991, The ORNL Modulating Heat Pump Design Model Tool—Mark IV user's Guide, ORNL/CON-343, Oak Ridge National Laboratory, Oak Ridge, TN.