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Laughman, C.R.; Qiao, H.; Nikovski, D.N.

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Kernel Regression for the Approximation of Heat Transfer Coefficients

Christopher R. Laughman^{*}, Hongtao Qiao, Daniel N. Nikovski

Mitsubishi Electric Research Laboratories
Cambridge, MA, USA
{laughman,qiao,nikovski}@merl.com

^{*} Corresponding Author

ABSTRACT

Experimentally-based correlations and other parametric methods for approximating heat transfer coefficients, while popular, have a number of shortcomings that are manifest when they are used in dynamic simulations of thermofluid systems. This paper studies the application of a nonparametric statistical learning technique, known as kernel regression, to the problem of approximating heat transfer coefficients for single-phase and boiling flows for the use in dynamic simulation. This method is demonstrated to accurately predict heat transfer coefficients for subcooled, two-phase, and superheated flows for a finite volume model of a refrigerant pipe, as compared to results obtained from established correlations drawn from the literature.

1. INTRODUCTION

Dynamic simulations of vapor compression systems, such as those used in refrigeration or air-conditioning applications, are an important tool for the processes of design, construction, and performance evaluation. Fast and accurate simulations enable explorations of the equipment design space more rapidly and at less cost than the comparable experimental work; moreover, the experimental exploration of larger systems is infeasible or impractical in many cases. Simulation tools can also be used to develop additional technology and functionality that augments and improves upon the design of the hardware itself, such as control systems or fault detection and diagnostic methods.

Although the systems of differential algebraic equations (DAEs) that represent the dynamic behavior of the system are mathematically and computationally complex, the underlying physics represented in the conservation equations is often well understood and can be expressed in a relatively straightforward and compact manner. In comparison, the set of closure relations, such as the interaction between the amount of heat transferred from the fluid and the temperature of the fluid, can seldom be accurately described in a succinct representation. These relations for the heat transfer coefficient α are often expressed through expressions such as $q = \alpha(\cdot)(T_1 - T_2)$, along with arguments of α that are determined by the particular application. While these heat transfer coefficients can be calculated analytically for a limited number of scenarios, the complexity of the boundary layer and turbulent transport precludes closed-form expressions for the heat transfer coefficients in many practical situations. Consequently, these relations are usually described with experimentally developed closed-form correlations for specific fluids and flow geometries of interest, which reduce the data using nondimensional numbers and other approaches to predict the heat transfer as a function of a relatively small number of available parameters.

Notwithstanding the popularity and simplicity of these heat transfer correlations, they have a number of limitations that warrant further consideration. In particular, the process of empirically determining the parameters of a given functional form that best fit experimental data will introduce errors between the datapoints and the resulting function; while these are inevitable, the errors between the data and the output of the functional form are not visible to a user of the correlation. It is important to note that such errors are avoidable in principle, while the measurement errors that occur during data collection due to experimental phenomena (e.g., sensor bias, experimental design) cannot

be mitigated in the fitting process without extra information. Second, the parameterization chosen for a given correlation might be susceptible to mathematical singularities and introduce nonlinear couplings between variables. While such limitations are often addressed in practice by the inclusion of additional constraints, these constraints often introduce numerical stiffness into simulations that can reduce robustness. This is a particular problem for models which operate on DAE system representations because of the challenges inherent in enforcing constraints on variables during the initialization process. Finally, these correlations are also often valid only for particular regions of flow, such as for single-phase turbulent flow or two-phase flow, necessitating the use of interpolation methods to piece together continuous functions over disparate regimes for dynamic simulations which include time-varying heat flows.

As this general problem of approximating the heat transfer coefficient from a chosen set of inputs can be viewed one of function approximation, a wealth of literature studying alternative approaches to the standard experimental correlation-based approach has emerged. The use of artificial neural networks (ANNs) from the machine learning community has attracted particular interest due to the flexibility of these methods for characterizing input/output behavior over a wide range of conditions for potentially large sets of inputs (also referred to as features). Mohanraj et al. (2012) recently surveyed the use of ANNs in a variety of different applications in the HVAC&R industry, and noted their particular successes in identifying complex nonlinear relationships between variables via the use of training data. More specifically, ANNs have been successfully used in the computation of two-phase heat transfer coefficients; Balcilar et al. (2011) used them to predict the condensing heat transfer of R134a in vertical smooth tube within 5% of experimental data, while Scalabrin et al. (2006) used them to predict the boiling heat transfer coefficients for a number of fluids within 10% and to identify flow pattern maps.

One key characteristic of these ANN methods is that they are parametric, meaning that the training process for the model of the heat transfer coefficient identifies a set of parameters intended to describe the training data. While this has such benefits as introducing bounds on size of a model, it can also result in undesirable behavior, such as the model becoming trapped in local minima due to the particular choice of the initial guesses for the parameters. Conventional methods of creating correlation functions are also susceptible to this problem, as described by Pacheco-Vega et al. (2001). This limitation is often addressed by use of very large sets of training data as well as global search methods, but the presence of sharp transitions in the underlying phenomena of interest, e.g., the change in the heat transfer coefficient as the fluid state moves from subcooled liquid to low quality two-phase fluid, can make the process of collecting sufficient experimental training data quite burdensome.

Nonparametric methods have a number of attractive features as alternative approach to the approximation of heat transfer coefficients. These methods build function approximations directly from the training data, rather than relying upon an intermediate training step. For example, a nonparametric approach to approximating a heat transfer coefficient will take measured heat transfer data and other system measurements, such as fluid density or the Reynolds number, and build a function approximator directly from these datapoints, rather than fitting the data to an intermediate functional form that will be provided to the final user. As a result, new data can be easily incorporated without the requirement for a new training step and the attendant modifications to the model structure. Because these methods are based directly upon the data, they are also not susceptible to local minima, and sufficient data in a region of interest will always improve the function estimate. The nonparametric nature of these models also ameliorates many of the problems that arise from mathematical singularities and limits on the validity of expressions because of the structure of the approximation method. Finally, data that is collected in the process of experimentally characterizing heat transfer coefficients is often captured in a tabular format, and can be included in such function approximators with a minimum of extra effort.

The work described in this paper is focused on studying and evaluating the performance of one nonparametric method, known as kernel regression, for approximating heat transfer coefficients in dynamic models of components in vapor compression systems. This method is studied by applying it to a dynamic heat exchanger simulation, written in Modelica (Modelica Association, 2014), using R290 as a working fluid. In Section 2 of this paper, we first motivate and describe some background of the kernel regression approximation method, and describe some

particular ways in which it was tailored to the problem of predicting heat transfer coefficients. While this kernel regression method has the capability of estimating heat transfer coefficients directly from experimental data, we evaluated its performance in this work via the use of existing correlations; we demonstrate the use of kernel regression on a dynamic pipe model in Section 3, first with a simple exemplar correlation that is conducive to visualization and then on a more complex correlation derived from the literature. Conclusions and perspectives for future work are finally reviewed and presented in Section 4.

2. KERNEL REGRESSION METHODS

Kernel regression is a nonparametric statistical learning technique that uses a family of local models of the training data, rather than a global model, to generate estimates y_0 at a query point x_0 . These local models are created from a weighting function $K_d(x_0, x_i)$, which prescribes the manner in which the contributions from datapoints x_i in a neighborhood of x_0 are combined to generate y_0 . The resulting output is smooth because of its use of local information around the entire neighborhood of the query point. These methods are often referred to as instance-based or memory-based methods because they compute estimates with little to no training computation; instead, all of the computation takes place when evaluating the function at the query point. The only parameter that must be determined is the width of the neighborhood d , which can either be specified statically or be adapted as a function of the data (Hastie et al., 2009).

This method generates its estimates by using a set of datapoints x_i in the domain $X \in \mathbb{R}^{N \times P}$ as well as a set of output values $f(X) \in \mathbb{R}^N$, where N denotes the number of datapoints and P denotes the number of features of the model. These datapoints are used to generate the estimate y_0 for the query point x_0 by computing a weighted average of all of the neighboring data points within a distance d of the query point, as in

$$\hat{f}(x_0) = \frac{\sum_{i=1}^N K_d(x_0, x_i) y_i}{\sum_{i=1}^N K_d(x_0, x_i)}. \quad (1)$$

This approach can be viewed as an extension of a moving average model, where the weighting function is used in the place of a uniform window to avoid the discontinuities that occur as datapoints enter and leave the averaging window.

The argument of the weighting function K_d is structured to use the distances between the query point x_0 and the data points x_i to evaluate the function, as

$$K_d(x_0, x_i) = T\left(\frac{|x_0 - x_i|}{d}\right). \quad (2)$$

A variety of distance functions and weighting functions have been successfully used for kernel regression (Atkeson et al., 1997); we used the standard Euclidean distance and the so-called tricube kernel in this work. This weighting function, given by

$$T(u) = \begin{cases} (1 - |u|^3)^3, & \text{if } |u| \leq 1 \\ 0, & \text{otherwise} \end{cases} \quad (3)$$

is appealing because it goes to zero outside the width d of the interval. Its smoothness ensures differentiability at the boundary of support, while its compactness causes the computation of the estimates to be zero outside of the distance to the query point and thereby facilitate sparsity in the computation. The resulting output is continuous and also has continuous first derivatives, though continuity is not guaranteed for higher derivatives.

Figure 1 illustrates the effect of using the kernel regression method to estimate the heat transfer coefficient generated from 24 datapoints obtained from an experimentally-based heat transfer correlation, described in §3.3. Because steady-state flow points were used to generate the data from which the estimate was constructed, the only feature used to estimate the heat transfer coefficient is the thermodynamic quality x_q of the refrigerant in the volume,

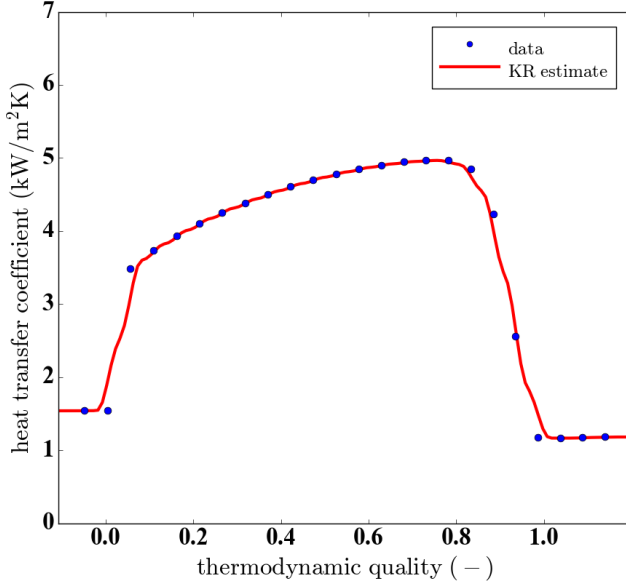


Figure 1: A 1D kernel regression example.

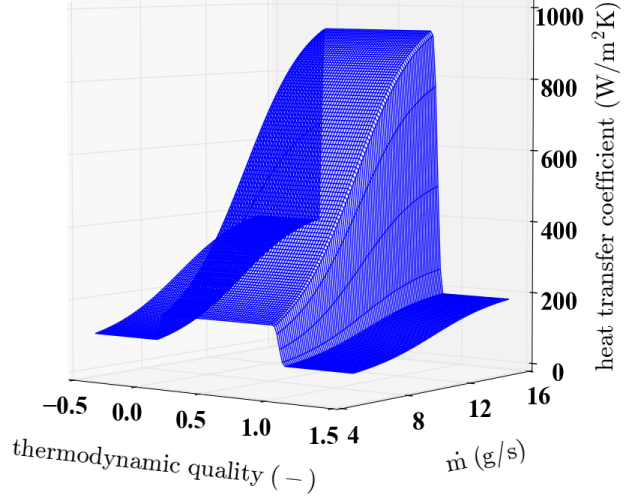


Figure 2: HTC surface as a function of \dot{m} and x_q .

defined as $x_q = (h - h_f)/h_{fg}$. It is apparent from this plot that the kernel regression estimate of the heat transfer coefficient closely follows the data provided, and that the resulting estimates for these flow conditions would accurately represent the measured data from the system.

This implementation of this kernel regression method requires the value of the neighborhood width d for the computation of the kernel weights. Rather than use a constant value of d , the distribution of datapoints can be taken into consideration by using a small value of d in regions of the data space where there is a high density of points, while increasing d in sparsely populated regions to ensure that a sufficient number of data points are used to generate the estimate. A K-nearest neighbors approach was employed to generate this set of distances; for each datapoint x_0 , the NN nearest neighbors were identified, and then the maximum Euclidean distance between x_0 and the other members of this nearest neighbor set determined the kernel width d_0 .

This method was also modified to adapt its behavior in regions outside of the neighborhood of collected data. Because the weighting function has compact support, the estimate of the heat transfer coefficient will go to zero outside of this neighborhood. While this behavior is useful in many machine learning applications, it is problematic for dynamic simulations because it will result in an adiabatic boundary condition where none is intended. When the query point is outside of the cloud of data points in this application, causing all of the kernel weights to be zero, we force the estimate to converge to the point on the boundary nearest to the query point by finding the point x_c that minimizes the Euclidean distance to the query point x_0 through a direct search of the N datapoints, and then using the corresponding closest data point y_c to modify Equation 1 so that the estimate smoothly goes to the value on the boundary, i.e.,

$$\hat{f}(x_0) = \frac{\sum_{i=1}^N K_d(x_0, x_i) y_i + \varepsilon y_c}{\sum_{i=1}^N K_d(x_0, x_i) + \varepsilon}. \quad (4)$$

A small value of ε (10^{-5}) is used so that this term does not add bias within the region where there is support from data while enabling $\hat{f}(x_0)$ to be nonzero outside of this region as well.

3. PIPE SIMULATION

A family of related dynamic pipe models were created to evaluate the performance of this new approach to describing heat transfer coefficients in simulation. All of these models were based upon a common finite volume model

of the fluid behavior in a pipe with a circular cross-section. Each of these models was then extended by using different functions to compute the heat transfer coefficients. The performance of the kernel regression method for estimating these heat transfer coefficients was then assessed by comparing the heat transfer coefficient generated by the kernel regression method to the analogous output produced by the different base heat transfer calculation functions. For the sake of simplicity, these simulations were only done for boiling flows, though we expect that condensing flows would behave similarly. In this section, we first describe the finite volume model used to describe the thermofluid behavior in the pipe in §3.1, and then describe the different heat transfer correlations used to evaluate the performance of the kernel regression method in §3.2 and §3.3.

3.1 Finite Volume Model

While a number of different modeling strategies are generally used to construct dynamic models of heat exchangers, we used finite volume models (FVMs) in this work because of their superior ability to characterize the spatially-dependent behavior of the heat exchanger. Because these FVM methods directly discretize the PDEs describing the conservation relations using the method of lines, model representations using this approach tend to result in large systems of equations with many states. A number of assumptions were thus used to simplify the model to avoid unnecessary model complexity in the models; these assumptions included one-dimensional pipe flow, instantaneous thermodynamic equilibrium in each control volume, the neglect of gravitational forces on the pressure drop, and homogeneous flow (equal phasic velocities) in the boiling region.

In consideration of these assumptions, the partial differential equations describing the conservation equations for a volume of working fluid can be discretized via the Reynolds transport theorem to generate a set of ordinary differential equations (ODEs), e.g.,

$$\frac{d(\rho_j V_j)}{dt} = \dot{m}_k - \dot{m}_{k+1} \quad (5)$$

$$\frac{d(\dot{m}_i l)}{dt} = \rho_j v_j^2 A_j - \rho_{j+1} v_{j+1}^2 A_{j+1} + \frac{A_j + A_{j+1}}{2} (P_{j+1} - P_j) + F_{f,i} \quad (6)$$

$$\frac{d(\rho_j u_j A_j)}{\partial t} = \dot{H}_k - \dot{H}_{k+1} + v_j A_j (P_{j+1} - P_j) + v F_{f,i} + \dot{Q}_j \quad (7)$$

where the symbols and nomenclature used in these equations can be found in the table at the end of this paper. The size of this set of ODEs corresponds to the number of discretized pipe volumes, and the indices refer the fact that we are using a staggered flow grid. In these equations, the i indices are referred to the momentum grid, the j indices are referred to the thermal grid, and the $k = j + 1$ indices refer to the boundaries of the thermal grid. In the models used for this work, we used 24 control volumes on the thermal grid. In addition, the term \dot{H}_k is defined as

$$\dot{H}_k = \dot{m}_k \bar{h}_{upstream,j}, \quad (8)$$

and the mixed-cup specific enthalpy \bar{h} is equal to the *in situ* specific enthalpy under the homogeneous flow assumption (Laughman et al., 2015).

Equations of state for the real fluid and a set of relations describing the closure relations are also needed to construct a complete system of equations that can be integrated forward in time. As R290 was used as the working fluid in these simulations, we used a set of state equations proposed by Span and Wagner (2003) for this fluid. We also used a simple equation to describe the relation between the mass flow rate of the refrigerant and the frictional pressure drop, as given by

$$\Delta P = K \frac{(\Delta P)_0}{\dot{m}_0^2} \dot{m}^2. \quad (9)$$

The nominal values of $(\Delta P)_0$ and \dot{m}_0 for this simple model were then included as parameters that were fixed when running the simulation. While this relation for the frictional pressure drop represents a significant simplification in

comparison to experimentally-observed phenomena, this relation was used to simplify the model so that dynamics due to the alternate heat transfer correlations could be better studied.

A number of ancillary models were also needed to construct a full simulation of the flow dynamics of the pipe. The above model of the refrigerant pipe was thus connected to a specific enthalpy and mass flow boundary condition on its upstream port and a pressure boundary condition on its downstream port. A heat flow boundary condition was also attached to every control volume of the pipe, allowing the heat flux to be varied. To study the system behavior, the mass flow rate of refrigerant through the pipe was increased from 5 g/s to 15 g/s at 200 seconds with a ramp of 100 second duration, and then the heat flux per control volume was increased at 500 seconds from 200 W to 250 W in a ramp, also of duration 100 seconds, so that the final total incident heat flux on the pipe was 6 kW. These simulations were implemented in the Modelica language, using the Dymola 2016 compiler, because the language enabled the closure relation describing the heat transfer coefficient to be replaced without affecting any of the code describing the rest of the model behavior, thereby facilitating a parametric exploration of model dynamics with a minimum of code modification.

3.2 Simple Heat Transfer Coefficient

The efficacy of the kernel regression-based heat transfer coefficients was first compared to a simplified heat transfer relation designed to facilitate direct visualization. As such, this heat transfer coefficient is specified only as a function of two variables: the mass flow rate and the thermodynamic quality of the refrigerant. A sigmoid function was used to allow the single-phasic heat transfer coefficient to smoothly vary between two constant values as a function of the mass flow rate, e.g.,

$$\alpha = \alpha_{min} + \frac{\alpha_{max} - \alpha_{min}}{1 + \exp(-k(\dot{m} - \dot{m}_0))}. \quad (10)$$

Three separate instances of this function were used to approximate the variation in the heat transfer over the three possible fluid phases, with different α_{min} and α_{max} values used for each phase. These functions were then combined into a single expression for the heat transfer coefficient by using a trigonometric interpolation scheme described by Richter (2008). The corresponding heat transfer coefficient surface is illustrated in Figure 2.

Because the kernel regression method constructs the estimate of the heat transfer coefficient at a query point from a combination of kernels, the selection of the kernel width d can have a significant effect on the estimates. As discussed in §2, we select the kernel width based upon the maximum distance in a neighborhood with NN nearest neighbors, where NN is chosen by the user. A small neighborhood size will increase the sensitivity to local variation, while a large neighborhood size will tend to include data from a wide range of conditions. We explored these tradeoffs by examining the performance of the method with 10, 20, 200, and 500 nearest neighbors.

We first ran an initial set of simulations with initial guesses for the constant phasic heat transfer rates that were far away from the actual heat transfer coefficients, and then we iteratively ran additional simulations to gradually construct the map of the heat transfer coefficient over the range of the variables manifest in the simulation. In all of the cases studied, only three simulations were necessary. The performance of the kernel regression method was validated by comparing the resulting estimates of the heat transfer coefficient to the output of a simulation that included the full heat transfer correlation.

As is evident from the results illustrated in Figure 3 (particularly the trace associated with $NN = 20$), the kernel regression method can accurately describe the heat transfer coefficient for a volume in the pipe over a wide range of inputs. While there are some errors near abrupt changes in the heat transfer coefficient, experimental values of the heat transfer coefficient are often characterized poorly around the saturation lines, so that the difference between these two datasets in these regions are small enough to remain negligible for most applications.

This figure also emphasizes the significant impact of the kernel width on the quality of the estimates. The small kernel widths generated by using 10 or 20 nearest neighbors produce estimates which are very close to the validation data set, while the larger kernel widths generated by using 200 or 500 nearest neighbors clearly do not perform as

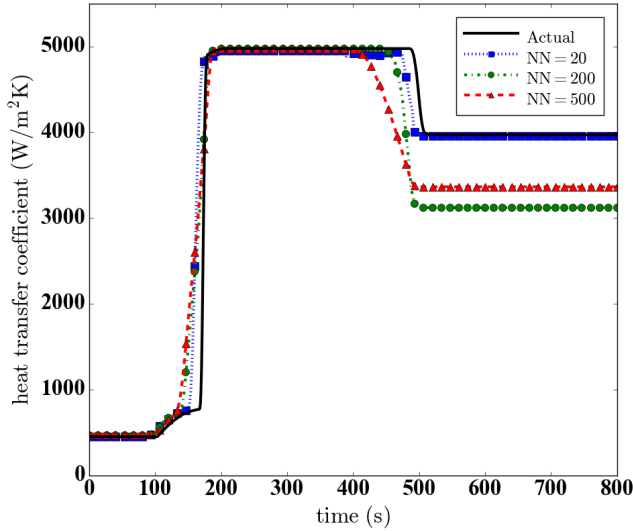


Figure 3: Simple HTC results.

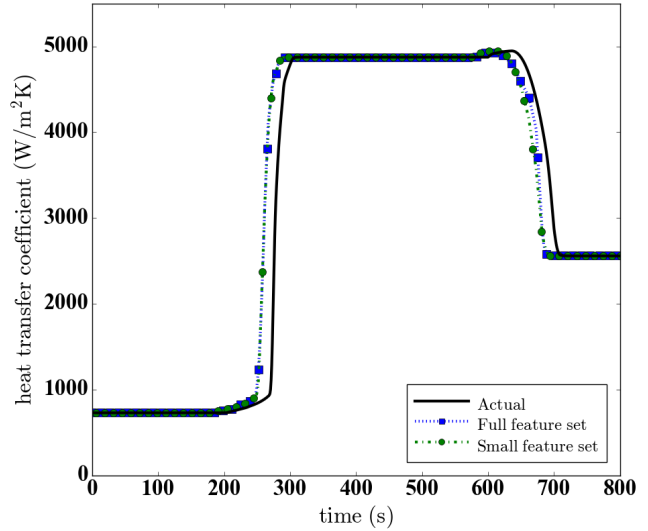


Figure 4: Experimentally-based HTC results.

well. This can also be seen in considering of the root mean squared errors; the RMSE of the heat transfer coefficient for the full set of 24 control volumes for 10 and 20 nearest neighbors are $297 \text{ W/m}^2\text{K}$ and $294 \text{ W/m}^2\text{K}$, respectively, while these values increase to $354 \text{ W/m}^2\text{K}$ for $\text{NN}=200$ and $638 \text{ W/m}^2\text{K}$ for $\text{NN}=500$. The large changes in value in the surface of the heat transfer correlation thus suggest that choices of fairly small neighborhoods are prudent in this application.

3.3 Experimentally-Based Heat Transfer Coefficient

Additional models and simulations were constructed to assess the accuracy of this approximation using experimentally validated heat transfer correlations. Such correlations for the different phasic regions were thus drawn from the literature and spliced together by the trigonometric interpolation scheme proposed by Richter (2008). The laminar and turbulent local Nusselt numbers for single phase flow were obtained by a set of correlations developed by Gnielinski (Stephan, 2010). These correlations, which apply for different ranges of Reynolds number, were themselves spliced together around the turbulent transition for Reynolds numbers between 3800 and 6100. The Gungor and Winterton (1987) correlation for boiling heat transfer for refrigerants was also used. A number of numerical regularizations were required to enable the use of this spliced correlations in Modelica to address initialization problems; for example, differentiable nonlinear limits were added to some of the terms to accommodate nonphysical input values that arise during initialization. The resulting simulation was nearly identical to that described in §3.2, the only difference being the use of the experimentally-based heat transfer coefficients, and was used to validate the performance of the predictions from the kernel regression method.

One important consideration for memory-based learning methods is the determination of the size of the feature set. While correlations that determine the phasic heat transfer coefficients use an array of geometric and thermodynamic parameters so that they can be used for a wide variety of systems and working fluids, specific system models are usually only concerned with a small subset of parameters because much of the geometric and thermodynamic information (e.g., channel diameter or working fluid) is constant over the simulation. We therefore constructed two feature sets to explore the sensitivity of the heat transfer coefficient to these selections. One of these feature sets included many of the parameters used in these correlations: Boiling number, Froude number, Prandtl number, Reynolds number, specific enthalpy and density of saturated liquid and vapor, thermal conductivity of the saturated liquid, local length in the direction of the flow, and the thermodynamic quality. In comparison, the second feature set only included the mass flow rate and the thermodynamic quality.

The results of applying kernel regression using both of these feature sets to approximating these complex heat transfer coefficients are illustrated in Figure 4. As with the previous set of simulations, it is evident that the kernel regression method describes the heat transfer coefficient quite well. The validation simulation using the complex heat transfer coefficient was very sensitive to the initial conditions due to the nonlinearities; in comparison, the simulation with the kernel regression method was much more robust to the initial conditions. Of particular note is the fact that both feature sets had nearly identical performance, as the RMSE for the full feature set was 259.05 W/m²K, while the RMSE for the restricted feature set was 259.41 W/m²K. This suggests that the actual heat transfer coefficient surface for a given model and related set of simulations lives in a space of much smaller dimension than is suggested by the number of parameters in the experimentally published correlations. This is particularly valuable information for the modeling process, suggesting that these simulations will result in smaller sets of nonlinear equations and faster computation time.

4. CONCLUSIONS AND FURTHER WORK

The initial results of using kernel regression methods to characterize and approximate heat transfer coefficients presented in this paper are quite positive, suggesting that these methods could be productively used in dynamic simulations of multiphase dynamic thermofluid simulations. While there are some small deviations between the heat transfer coefficients predicted by conventional approaches and those predicted using the kernel regression methods, the regions in which these errors are located are generally susceptible to relatively high experimental uncertainty, and both methods can produce comparable estimates in regions that are not near the saturation lines. These kernel regression methods are not susceptible to some of the shortcomings of parametric heat transfer approximation methods, and can be potentially used to reduce the computational complexity of models and simulations because of their ability to describe relevant phenomena in a smaller feature space than is often used. They also have the advantage of being easily extensible; additional heat transfer data can be incorporated into the approximation method with a minimum of effort, effectively creating low-dimensional correlations that are customized to a particular application.

A number of excellent opportunities remain for further work and study. Two immediate areas of future work include the application of these methods to condensing flows, as well as the application of analogous methods to the estimation of frictional pressure drops in standalone applications and in complete cycles. Studies of these and other related topics could present new and exciting opportunities for advancing the state-of-the-art in dynamic system simulation by reducing computation time and increasing simulation accuracy and robustness.

NOMENCLATURE

A	cross-sectional area	h_{fg}	specific enthalpy of vaporization
\dot{H}	mass flow rate-weighted enthalpy	\bar{h}	mixed-cup specific enthalpy
NN	nearest neighbor	l	cell volume length
P	pressure	\dot{m}	mass flow rate
Q	heat flow rate	q	heat flux
T	temperature	u	specific internal energy
V	cell volume	v	velocity
h	<i>in situ</i> specific enthalpy	x_q	thermodynamic quality
h_f	specific enthalpy on saturated liquid line	α	heat transfer coefficient
h_g	specific enthalpy on saturated vapor line	ρ	density

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