STRUCTURE-BASED GENERALIZED MODELS FOR SELECTED PURE-FLUID SATURATION PROPERTIES

By

AJAY JEGADEESAN

Bachelor of Engineering (Honors)

Birla Institute of Technology and Science

Pilani, Rajasthan (India)

May 2003

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
the requirements for
the Degree of
MASTER OF SCIENCE
December, 2006

STRUCTURE-BASED GENERALIZED MODELS FOR SELECTED PURE-FLUID SATURATION PROPERTIES

Thesis Approved:

Khaled A.M. Gasem

Thesis Adviser

Martin. S. High

Robert L. Robinson, Jr.

A. Gordon Emslie

Dean of the Graduate College

PREFACE

This study focused on developing generalized structure-based models for predicting pure-fluid surface tensions and saturation viscosities. Reliable experimental data for a wide range of molecular species were assembled from the DIPPR physical property database. The Scaled-Variable-Reduced-Coordinate (SVRC) framework was used to correlate the available data for the saturation properties under consideration. Quantitative Structure-Property Relationships (QSPR) was used to generalize the SVRC model parameters. Non-linear QSPR models involving a hybrid of Genetic Algorithms (GA) and Artificial Neural Networks (ANN) were developed for the model parameters.

The hypothesis for this work was that an approach that calls for the use of theory to develop the behavior model, and QSPR to generalize the parameters of such model, is more effective than attempting to model the properties directly using QSPR. The quality of the predictions obtained for a diverse group of molecules demonstrates the validity of this integrated approach and provides credible evidence to support the above hypothesis.

Specifically, the SVRC-QSPR models, in general, were found to be capable of providing generalized *a priori* predictions for surface tension and saturation viscosities with an absolute average deviation (AAD) of approximately 2% using end-point input data.

ACKNOWLEDGEMENTS

I thank all my teachers, colleagues, and friends who have been associated with me throughout the course of my graduate study. My sincere thanks to Dr. Khaled Gasem for providing me with this learning opportunity and guiding me through it. I would also like to thank my committee members, Dr. Robert Robinson and Dr. Martin High for their guidance and valuable suggestions. Special thanks go to Dr. Srinivasa Godavarthy and Eric Whitebay for their help. Finally, I would like to thank my family members for all their support.

TABLE OF CONTENTS

Chapter **Page**

LIST OF TABLES

Chapter 2 SVRC-QSPR Model for Liquid Viscosities

Chapter 3 SVRC-QSPR Model for Vapor Viscosities

Chapter 4 SVRC-QSPR Model for Surface Tensions

LIST OF FIGURES

Chapter 2 SVRC-QSPR Model for Liquid Viscosities

Chapter 3 SVRC-QSPR Model for Vapor Viscosities

Chapter 4 SVRC-QSPR Model for Surface Tensions

NOMENCLATURE

Symbols

AAD	absolute average deviation
A,B,C	correlation constants
P	parachor
RMSE	root-mean-square error
T	temperature
T_c	temperature at critical point
T_t	temperature at triple point
TR	training set
PR	prediction set
Y	saturation property

Greek Symbols

α	scaling exponent
α_c	scaling exponent at the critical point
α_t	scaling exponent at the triple point
$\Delta\alpha$	$(\alpha_{c} - \alpha_{t})$
ε	$(T-T_c)/(T_c-T_t)$
Θ	correlating function
$\omega^{2,2}$	collision integral
η	viscosity
σ	surface tension
σ_r	reduced surface tension
ρ_L	liquid density
ρ_V	vapor density
ρ_{Lb}	liquid density at boiling point

Subscripts and Superscripts

c	critical point state
calc	calculated
exp	experimental
r	reduced property
rep	reported
t	triple point state

CHAPTER 1

INTRODUCTION

Accurate knowledge of thermo-physical properties of pure gases, liquids, and their mixtures is essential for chemical process design. Errors in the values of these properties can have a significant impact on the engineering design and can also lead to unexpected increases in the operating costs. Also these errors can propagate throughout the design of the entire plant and may become amplified and threaten operability. Along with the demand to optimize existing processes, an increasing need also exists for the design of new cost-effective processes and the synthesis of new improved materials. The traditional approach has been to determine the properties of these new materials experimentally. However, experiments can be time consuming and expensive. An alternate approach is to use thermo-physical property estimation methods. A viable estimation method should have the following attributes: (1) be applicable to a diverse set of compounds; (2) be applicable over a wide range of temperatures and pressures; (3) require a minimum number of input parameters; (4) provide the probable confidence in the predicted property; (5) provide reasonable accuracy relative to expected experimental uncertainty; and (6) require minimum computation time [1].

Several prediction methods are often available to estimate a given thermo-physical property for a specific group of compounds. However, as the heterogeneity in the molecular structure of the compounds increases, property prediction becomes less reliable and more time consuming [1]. Several approaches are generally used for estimating thermo-physical properties, including: correlations (empirical, semi-empirical, and theoretical) based on limited experimental data, group-contribution methods (i.e., atom, molecular fragments), quantitative structure-property relationships (QSPR), theoretical models (e.g., equations of state), and molecular simulations. Correlations requiring properties as input (such as boiling point temperatures, melting point temperatures, or critical properties) are limited to compounds for which such experimental data exist. Group-contribution methods can be applied to compounds when the contribution parameters of chemical bonds, functional groups and/or atom types for the compound of interest are available. They become less reliable for predicting properties of compounds with multiple functional groups and for isomers [1]. Hence there is a need for reliable generalized property models capable of *a priori* predictions of pure-fluid properties of diverse systems, thereby reducing the burden of experimentation.

The need for specialized correlations for each saturation property amplifies the usefulness of a unified and generalized framework for the prediction of pure-fluid saturation properties. Researchers at Oklahoma State University (OSU) have developed the scaled-variable-reduced-coordinate (SVRC) model [2, 3], based on corresponding states theories (CST) and scaling laws. This model has provided precise representations of pure-fluid behavior. Initially, generalized equations for the model parameters were developed based on traditional physical properties (e.g., boiling point, acentric factor, etc.). The SVRC model provided accurate predictions for normal fluids. The results obtained indicated that the trends produced by the SVRC model parameters can be used in developing a reliable predictive model. However, generalizations for polar fluids were less accurate, as the model generalizations did not account for the structural variations of the different classes of compounds [3]. To overcome this problem, a different generalization strategy was sought. Recently, Quantitative Structure-Property Relationships (QSPR) modeling has proven to be effective in correlating the properties of compounds in terms of their structures. The approach is based on a premise that any property associated with the compound is encoded in its chemical structure. QSPR provides information on the influence that the structure of a compound has on its properties. However, most QSPR correlations have been based on multiple regression correlations requiring *a priori* assumption of the mathematical form of the correlation model. Such models do not consider the non-linearity that may exist among the input and the output parameters. Also, most current QSPR models are limited to predictions at a single temperature, and a need exists to extend this structure-based modeling to describe the entire saturation range. To overcome the drawbacks of conventional QSPR models, an approach that involves the use of QSPR methodology to generalize the model parameters of the developed SVRC model was proposed by previous researchers at OSU [4, 5]. In this approach, SVRC model was used to represent accurately the behavior of the data, and QSPR was used to generalize the parameters in the model. In previous studies, this approach proved to be more effective than the typical efforts to develop generalized models directly using QSPR techniques [4, 5].

Objectives

The goal of this research was to develop structure-based generalized models for the *a priori* prediction of: (a) pure-fluid saturation phase viscosities and (b) pure-fluid surface tensions. The specific objectives for accomplishing this goal were to:

1. Compile a reliable database of pure-fluid saturated phase viscosities and surface tensions for model development and validation.
2. Extend the SVRC framework to correlate available data for the saturation properties under consideration.
3. Build non-linear QSPR models to provide structure-based parameters for the SVRC model.
4. Determine the efficacy of QSPR generalized models in providing *a priori* predictions of the saturation properties considered within two to three times the experimental uncertainty.

Thesis Organization

This thesis is written in the "manuscript style," and it is divided into three separate self-contained manuscripts. Since the same modeling strategy was adopted for all three saturation properties under consideration, some sections of the individual chapters may appear repetitive. Also, the modeling methodology used in this study has been developed in collaboration with other members of the OSU Thermodynamics Research group [4, 6]. Consequently, similar documentation has been used. Chapters 2, 3, and 4 deal with the methodology adopted and the results obtained for modeling liquid viscosity, vapor viscosity, and surface tension, respectively. Conclusions based on the efforts undertaken and suggestions for future directions for research are given in each of these chapters.

References

1. Yaffe, D.L., A Neural Network Approach for Estimating Physicochemical Properties Using Quantitative Structure-Property Relationships (QSPRs), University of California: Los Angeles, Ph.D. Thesis, 2001.

2. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Vapor Pressures. Fluid Phase Equilibria, 1991. 64: p. 141-163.

3. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Liquid Density. Fluid Phase Equilibria, 1992. 64: p. 81-98.

4. Ravindranath, D., Structure-Based Generalized Models for Pure-Fluid Saturation Properties and Activity Coefficients, Oklahoma State University: Stillwater, M.S. Thesis, 2005

5. Godavarthy, S., R.L. Robinson, Jr., and K.A.M. Gasem, SVRC-QSPR Model for Predicting Saturated Vapor Pressures of Pure Fluids. Fluid Phase Equilibria, 2006, 264: p. 39-51.

6. Godavarthy, S., Design of Improved Solvents for Extractive Distillation, Oklahoma State University, Ph.D. Dissertation, 2004.

CHAPTER 2

SVRC-QSPR MODEL FOR LIQUID VISCOSITIES

Introduction

Viscosity is an important transport property used in engineering design for transportation and processing of fluids. Techniques for measuring the viscosities of fluids have been available for many years. Despite their widespread use, however, many of them are time-consuming, expensive, and unreliable. Operational and maintenance problems plague the process of making experimental viscosity measurements [1]. These problems are further amplified in the case of hazardous chemicals where handling and storage cause problems.

Although conducting experimental measurements is still the preferred (most accurate) method for determining the viscosity of many fluids, reliable models capable of providing a *priori* predictions would certainly supplement the process, especially when dealing with new and challenging chemicals. Currently, many correlations for estimating liquid viscosities are available in the literature. However, most of these correlations have a limited range of applicability and poor suitability for generalization.

Generalizations made using these traditional physical properties do not capture the subtleties of various chemical structures and, hence, provide poor predictions. Moreover, the values for these physical properties are not available for numerous new and structurally complex molecules. Quantitative structure-property relationship (QSPR) models offer an attractive alternative since they have the potential to provide reliable property estimates based on chemical structure information alone. Literature studies which use structural descriptors for correlation of liquid viscosities have been published. However, currently available QSPR models for liquid viscosity are limited to predictions at a single temperature and/or are restricted to a narrow range of chemical species. Also, most of these models use experimentally determined physical properties (e.g., critical temperature, normal boiling point, etc.,) as descriptors and hence are restricted to compounds for which these data are available (see, e.g., [14]).

Previously, researchers at Oklahoma State University (OSU) have developed a unified framework for correlating saturation properties, which include vapor pressure and liquid and vapor densities [2, 3]. This scaled-variable-reduced-coordinates (SVRC) framework is based on the corresponding states theory (CST) and scaling-law behavior, and, in general, it is capable of representing saturation properties within their experimental uncertainties. In this work, the SVRC model is extended to correlate liquid viscosities in the saturated region and the model parameters are generalized using structure-property modeling.

A database of 1345 data points involving 78 fluids was used to develop the model, and an external dataset containing 16,383 data points involving 638 fluids was used for secondary validation. The approach involves using QSPR methodology to generalize the model parameters of the developed SVRC model; thus, we use the SVRC model to correlate the liquid viscosities, and QSPR to generalize the parameters in the model. This approach, in the past, has proven to be more effective than the typical efforts to develop generalized models directly between the property and its descriptors using QSPR techniques (see, e.g., [4]).

Liquid Viscosity Prediction Models

Estimation of viscosity for organic compounds that are yet to be synthesized requires reliable generalized predictive models. Viscosity of gases is well described by the kinetic theory. However, for dense gases and liquids, due to the existence of a wide variety of intermolecular forces and degree of disorder among the molecules, a theoretical description is difficult. Several models for predicting viscosities of dense gases and liquids are available in the literature. A comprehensive review of some of these commonly used models is provided by Reid and co-workers [5] and Monnery and co-workers [6]. The models for prediction of liquid viscosity can be classified into theoretical, semi-theoretical and empirical models. The theoretical models are mostly based on statistical mechanics and molecular dynamics simulations. These models give rise to large deviations in predictions which preclude their usage.

The semi-theoretical models have been based mostly on the following: corresponding states principle, reaction rate theory, hard sphere theory, square well theory, modified Chapman Enskog theory, free volume model, friction theory, Eyring's absolute rate theory and significant structure theory. Monnery and co-workers [6] provide a comprehensive review of the theory behind these models and their applicability. Apart from the approaches mentioned above, models that are strictly empirical are available in abundance in the literature. A comprehensive review of some of the most commonly used empirical models are summarized in detail elsewhere [6]. Recent literature efforts have centered on modifications to absolute rate theory [7, 8], square well model [9], friction theory [10], corresponding states principle [11], and significant structure theory [12].

A majority of the literature models rely on experimentally-measured physical properties as input for their predictions. Although experimental data are available in the literature for numerous compounds that have been already investigated, there arises a need for a generalized model capable of providing *a priori* predictions for compounds that are yet to be synthesized. This requires the establishment of a relationship between the viscosity of the liquid and its chemical structure. The use of quantitative structure-property relationship (QSPR) is one such approach where models are obtained on the basis of the correlation between the experimental values of the property and descriptors reflecting the molecular structure of the respective compounds.

Suzuki and co-workers in 1996 proposed the use of QSPR approach for prediction of liquid viscosities [13]. Their approach assumed that the relationship between experimental liquid viscosities and the other physicochemical properties or numerical molecular descriptors can be expressed in the following multi-linear form:

$$\log \eta_i = \sum_{i=1}^{n} a_i X_{ij} + C_0$$

where log η_i is the logarithm of the liquid viscosity of compound j, a_i is the coefficient of the ith descriptor X_i**,** n is the number of descriptors in the model and C_o is a constant. Using a combination of partial least-squares (PLS) and QSPR techniques, they developed a nine-descriptor model which included four key physical properties (molar refraction, critical temperature, molar magnetic susceptibility, and cohesive energy), and five structural descriptors. A set of 237 compounds having diverse structures containing C, H, N, O, S, F, Cl, Br and I were used in the study which gave a squared correlation coefficient (R^2) of 0.92 and a root-mean-square error (RMSE) of 0.17 log mPa.S.

Again in 1997, Suzuki and co-workers [14] extended their multi-linear model by including another 124 compounds and developed an alternative approach for predicting liquid viscosity by applying neural network (NN) techniques. The non-linear model had a R^2 value of 0.93 and an RMSE of 0.16 log mPa.S for a prediction set of 124 compounds. Based on the work of Suzuki and co-workers, Katritzky and co-workers developed a QSPR model for predicting viscosities of a diverse set of compounds utilizing the CODESSA descriptors derivable solely from the structure of the compounds [15]. They investigated the liquid viscosities of 361 organic compounds containing C, H, N, O, S and halogens and proposed a five-descriptor equation with a R^2 of 0.854 and a standard error (S) of 0.22 log mPa.S.

The above QSPR models are successful only in predicting the liquid viscosities at one particular temperature (20 ^{0}C). A thorough review of the literature suggests that most of the predictive methods found in the literature are restricted to a narrow range of compounds and temperatures. However, a few of them are generalized and are applicable over the entire saturation range. Further, the accuracy and reliability of these models are difficult to state because (a) the testing methods adopted by the different authors lack a common database, (b) the range and applicability of the testing has not been stated in the literature [6], and (c) most of these models present large deviations in the near critical region. Hence, there is a need for a generalized model utilizing a minimum number of parameters capable of predicting fluid viscosities over a wide temperature range and for a diverse set of compounds.

Scaled-Variable-Reduced-Coordinate Framework

In previous studies [2, 3], the SVRC framework was used to correlate saturation properties of a wide variety of organic molecules over the entire saturation range. The general SVRC framework for correlation of thermo-physical properties is given as [2, 3]:

$$\left(Y_{\infty}^{\alpha} - Y^{\alpha}\right)/\left(Y_{\infty}^{\alpha} - Y_{0}^{\alpha}\right) = \Theta(\varepsilon) \tag{1}$$

or

$$Y^{\alpha} = Y_{0}^{\alpha}\Theta(\varepsilon) + \left[1 - \Theta(\varepsilon)\right]Y_{\infty}^{\alpha} \tag{2}$$

where

$$\varepsilon = \left(X_{\infty} - X\right)/\left(X_{\infty} - X_{0}\right) \tag{3}$$

$\Theta(\varepsilon)$ is the correlating function, X is the correlating variable, Y is the saturation property at given X, Y_{∞} is the asymptotic value of saturation property at X_{∞}, Y_0 is the initial value of saturation property at X_0 and α is the scaling exponent.

To correlate saturation properties, Equation (1) is recast for representing the various properties between the triple and the critical points as:

$$Y = \left\{Y_{c}^{\alpha} - \left(Y_{c}^{\alpha} - Y_{t}^{\alpha}\right)\Theta\right\}^{(1/\alpha)} \tag{4}$$

Applied specifically to liquid viscosity correlation, the above equation is written as:

$$\eta = \left\{\eta_{c}^{\alpha} - \left(\eta_{c}^{\alpha} - \eta_{t}^{\alpha}\right)\Theta\right\}^{(1/\alpha)} \tag{5}$$

where, η_c and η_t are the critical and triple point viscosities, respectively. In this work, due to restricted availability of data, the liquid viscosity data at the lowest and the highest temperatures available were taken to be η_c and η_t for modeling purposes.

The functions $\Theta(\varepsilon)$ and α are defined as:

$$\Theta(\varepsilon)=\frac{\left(1-A^{\varepsilon^B}\right)}{(1-A)} \tag{6}$$

$$\alpha=\alpha_c-\Delta\alpha\frac{\varepsilon(1+C\varepsilon)}{1+C} \tag{7}$$

Where

$$\varepsilon=\frac{T_c-T}{T_c-T_t} \tag{8}$$

and

$$\Delta\alpha=(\alpha_c-\alpha_t) \tag{9}$$

A, B and C are correlation constants, and α_c and α_t are the limiting values of α at the critical temperature and triple point temperature, respectively. The SVRC model accounts for the effects of temperature and chemical structure through the correlating function (Θ) and the scaling function (α). In the current study, the value of $\Delta\alpha$ in Equation (7) is taken to be zero (or $\alpha_c = \alpha_t = \alpha$); thus, a single-parameter model is used.

QSPR Methodology

Computational techniques have gained popularity recently owing to the advances in technology. They are increasingly used to address complex engineering and design problems in chemical processing. The QSPR approach is among the computational methods gaining wide use. It is based on the assumption that a relationship exists between the structure of a substance and its physical and chemical properties. QSPR uses quantum mechanics to define the structure of the molecule in terms of a series of molecular descriptors and then correlates the property in terms of these descriptors. The following steps are part of any QSPR model development effort [16]: (a) generation of 3-D structures, (b) optimization of 3-D structures, (c) calculation of descriptors, (d) reduction of descriptors, and (e) development of a QSPR model. Figure 2.1 outlines the procedure followed in the QSPR modeling effort undertaken. The procedure used to develop QSPR generalization for the SVRC model parameter (α) are outlined in the following paragraphs.

Database Development

A property database of pure fluids including alkanes, refrigerants, aromatics and alcohols was used in the SVRC model development for saturated liquid viscosities. The data used in this study were compiled mainly from the DIPPR database [17]. The DIPPR database, on the whole, contained 32,591 liquid viscosity data points involving 1200 fluids. This database was screened to include only organic compounds for which quality experimental data (with reported errors of less than 5%) were available. Also, only datasets with more than eight data points were included in the model development procedure. The screened database contained over 1435 saturated liquid viscosities data points involving 82 fluids. To the extent possible, for each compound, we sought data that covered a wide temperature range in the saturation region. Regression results for the SVRC model were used to identify data points with percent absolute average deviations (% AAD) greater than twice the overall regression %AAD of a compound; these points were then removed from the database in an effort to remove data with relatively large uncertainty. Based on this procedure, a total of 90 data points were eliminated which constituted about 6.3% of the total. The reduced database finally contained 1345 data points involving 78 fluids. A list of the compounds used and the reduced temperature ranges for each molecule can be found in Table A.1 of Appendix A. The final data set is more restricted than desired because currently, limited experimental data are available in the literature for viscosities. Even when available, they are often limited to a single temperature (298 K) or a narrow temperature range. Further, reliable data near the critical point are nearly non-existent. This may be attributed to the practical difficulties in measuring viscosity near the critical point.

Structure Generation

The first step in any QSPR modeling effort is the generation of chemical structures. Various kinds of chemical representation have been proposed in the literature. The most common way of representing a chemical is a two-dimensional (2-D) sketch [16]. However, using a 2-D representation does provide a complete description of the molecule and cannot be used conveniently for database storage and searching [16]. To have an efficient QSPR model, the representation of a molecule should provide all the necessary structural information. This requires information about the atoms present, along with three-dimensional (3-D) coordinates that provide a full spatial depiction of the molecule. A commercial package, ChemDraw [18] was used to generate the 3-D structures of the molecules.

Structure Optimization

More than one set of 3-D coordinates can be generated for any given molecule. Most molecules contain single bonds that join two atoms. Such bonds can usually rotate with a low-to-moderate energy barrier that changes the orientation of other atoms in the structure and thereby the value of the descriptors [16]. In nature, all these representations occur in differing probability and structure optimization must obtain a 3-D structure which is most prominent and has the minimal potential energy surface. In this work, the 3-D structures generated were first optimized using the MOPAC routine available in the ChemDraw package and later commercial optimization software called AMPAC [19] was used. The use of two optimization routines practically eliminated any un-optimized structures. Description of the intricate details of 3-D structure generation and optimization are beyond the scope of this work. More complete discussions can be found elsewhere [16, 19].

Descriptor Generation

Once an accurate 3-D structure of a chemical has been obtained, the next step involves calculation of the molecular descriptors. The molecular descriptors calculated by any commercial package are usually divided into (1) constitutional, (2) topological, (3) geometrical, (4) electrostatic, (5) quantum-chemical and (6) thermodynamic. Details about these classes of descriptors can be found elsewhere [16]. In this work, commercial software called CODESSA [20] was used to generate the descriptors. Around 400 descriptors were generated for each molecule. The actual number of descriptors calculated for each molecule varied based on the structural complexity of the molecule.

Descriptor Reduction

Many of the 400 descriptors generated for each molecule are not significant in modeling liquid viscosities. The use of all available descriptors in the model development effort causes dimensionality problems. Further, the use of irrelevant or redundant descriptors diminishes the performance of a QSPR model, especially when non-linear algorithms are used in model development. Descriptor reduction (DR) is the process of automating the discovery of potentially useful correlations from large sets of descriptors [16]. The DR process involves the identification of the most relevant set of descriptors for model development and is the most important step in all QSPR model development efforts. Several different methods for DR are available in the literature. The most widely used techniques are the principal-component analysis (PCA), partial least-squares (PLS), genetic algorithms (GA), and neural networks (NNs) [16].

Most QSPR models developed have been based on multiple linear regression correlations requiring *a priori* assumption of the (linear) form of the mathematical correlation model. Such models do not consider the non-linearity that may exist among the input parameters (descriptors) and the calculated property. The above deficiencies have been addressed in the past using Artificial Neural Networks (ANN). Neural networks are powerful tools for correlating, predicting and classifying large complex data sets. They can deal successfully with non-linearity, handle noisy or irregular data, correlate hundreds of variables or parameters, and provide generalized solutions [21]. However, commonly-used neural network architectures, such as back propagation networks, demand extensive training (using a significant amount of data) to develop a stable QSPR model [22]. This places further demand on modeling efforts since reliable experimental data are not easily available. Another Artificial Intelligence (AI) tool that has been used in QSPR model development is Genetic Algorithms (GA) [23, 24]. Genetic search methods are based on Darwinian models of natural selection and evolution. The general idea behind genetic algorithms is the evolutionary creation of a new population of entities from an earlier generation through crossover and mutation processes and by passing on the fittest offspring to the next generation [25]. This approach is ultimately expected to lead to generations that become fitter through evolution thereby achieving the desired objective. More details on GA can be found elsewhere [25].

Hybrid approaches using genetic algorithms and neural networks have also been recently proposed and have shown good promise in developing accurate and robust QSPR models [26, 27]. In this work, such a hybrid approach employing Genetic Algorithms and Neural Networks was used to develop a generalized non-linear model for liquid viscosities.

QSPR Model Development

This work aimed at (a) demonstrating the ability of the SVRC model to precisely represent saturated liquid viscosities using one regressed parameter, (b) examining the efficacy of using QSPR algorithms to obtain estimates for SVRC parameter based on chemical structure information using non-linear algorithms. Two case studies were conducted in sequence to achieve these objectives:

Case 1. Determination of the SVRC parameter (α) by regressing experimental data

Case 2. Generalization of the SVRC parameter using non-linear structure-based models

The liquid viscosity model development was initiated with the regression of the SVRC parameter (α) for each molecule (Case 1). As can be seen from Equations 5-7, SVRC model for liquid viscosity has five parameters A, B, C, α_c, and α_t. Since, in the current study, the value of $\Delta\alpha$ (in Equation 7) is taken to be zero (or $\alpha_c = \alpha_t = \alpha$), the model becomes a four-parameter model. Among these, A, and C are treated as universal constants applicable to all fluids. Based on regression, the values of these constants are fixed to be the following: A=1.33; C=0. B is the universal scaling exponent, which characterizes the divergence of viscosity near the critical point. Several values for this exponent have been proposed in the literature. A comparative study of these values is presented in Table 2.1. However, when the exponent values suggested in the literature were used for fitting the available experimental data, large errors were obtained. Therefore, based on subsequent regressions, a value of 1.0 for B was selected for use with the two universal constants (A=1.33; C=0), and the adjustable parameter (α). As shown in Figure 2.2, this combination provided good representation of the data. The figure shows how well the model represents the data using a combination of the constants suggested above. The lack of experimental viscosity data close to the critical point precluded us from determining a precise value for the critical exponent B that is reconcilable with the values proposed in the literature.

Structure-based model development for the model parameter (α) was initiated with structure generation, optimization, and descriptor generation. Studies have shown that structural descriptors are often highly correlated, leading to numerical instabilities commonly referred to as multicollinearity. In such instances, this causes increasing difficulty in disentangling the unique effects of each predictor (descriptor) on the response variable. Multicollinearity results in highly unstable estimated regression coefficients, the values of which are extremely sensitive to addition/removal of variables or small changes in data points leading to erroneous results and interpretations [28]. To tackle this problem, the use of orthogonal molecular descriptors has been suggested. The procedure of orthogonalization focuses on the residuals of intercorrelation between descriptors thereby ensuring that distinct structural characteristics of various descriptors are extracted and used as novel descriptors, which are free from mutual relatedness [28]. More information on the procedure of orthogonalization and its use can be found elsewhere [28, 29]. In this work, the descriptors generated by CODESSA were orthogonalized to obtain a subset of descriptors from which all redundant information has been removed. Non-linear DR techniques were then applied to this reduced subset of descriptors.

The non-linear modeling was performed using commercial software [30]. The reduced subset of descriptors obtained from the orthogonalization step is exported to the software which has a Microsoft Excel™ interface. The software employs a Genetic Algorithm (GA) to identify the best set of input variables for the model. A GA operates on a population of individuals. The population changes from one generation to the next, usually by combining characteristics of two "parent" individuals to create a "child" individual. Every individual is assigned fitness and the concept of "survival of the fittest" is implemented by selecting the fit parents more frequently than less fit parents to create the next generation [30].

In this case, an "individual" is actually a set of descriptors. The fitness of a descriptor is derived from the performance of a model that uses the descriptor's variable set as inputs. The algorithm begins with descriptors that consist of small sets of variables. Descriptors that produce good models are kept in the population and used to generate descriptors that consist of larger sets of variables if necessary. In general, however, smaller variable sets (that is, fewer model inputs) are preferred to larger variable sets. The fitness of a descriptor (set of descriptors) is evaluated using Neural Networks. The software constructs the actual neural network incrementally, using a technique known as cascade correlation. Hidden units are periodically added, usually one or two at a time. Each time a hidden unit or pair of hidden units is added, weights are trained from several different initialization values. Each initialization is referred to as a candidate. The best candidate is established in the network, and then all the weights to the output node(s) of the network are retrained.

There are several heuristics that provide guidance to the permissible number of hidden neurons or choice of networks weights and criteria for termination of training. For example, when determining the network architecture, the rule of thumb is to keep the ratio of total observations (number of molecules) to adjustable parameters (network weights) above two to avoid any chance effects. However, these rules are just for guidance and trial-and-error investigation remains the reliable method for choosing the optimum parameters [4]. To construct the neural network model, the data set containing 78 molecules were randomly split into training and prediction (test) sets. The training and prediction sets contained 70% and 30% of the data, respectively. After rigorous trial-and-error analysis, a neural network was developed for the SVRC model parameter (α). Specifically, an 8-3-1 (8 descriptors - 3 hidden neurons - 1 output variable) architecture was obtained using the training set. The SVRC parameters for the prediction set were then generated using the 8-3-1 network. The efficacy of the neural network model, as indicated by its accuracy and stability, is evaluated based on the quality of the model predictions (overall % AAD) obtained from the SVRC model as given by Equation 5.

Results and Discussion

Table 2.2 presents the summary results for the case studies conducted. The entire data set containing 78 molecules was correlated using a one-parameter SVRC model. As indicated by the results for Case 1, the SVRC model represents the liquid viscosities of the diverse organic subset over a wide temperature range in the saturation region, with AAD of 0.7% using one regressed parameter.

The SVRC parameter (α) was then generalized using non-linear QSPR models (Case 2). A hybrid approach employing Genetic Algorithms and Neural Networks was used to identify the best non-linear model that provided accurate predictions. GA was used to identify the best subset of descriptors and NN was used to evaluate the fitness of the selected individuals (descriptors). A sigmoidal transfer function [30] was used and several architectures were investigated by varying the number of hidden neurons. An 8-3-1 architecture for the parameter α was found to provide the best performance as measured from the overall fit (%AAD) of the property predictions from the model. The number of adjustable parameters in the network architectures was also found to obey the above mentioned heuristic (ratio of number of systems used for training to the number of adjustable parameters being greater than two). The descriptors generated from the non-linear model are presented in Table 2.3.

The generalized parameters obtained from the non-linear QSPR models are plotted against the regressed values in Figure 2.3. The plot shows the efficacy of the neural network model in predicting the parameters. Nonetheless, the limited data available for training constrained the model development efforts resulting in poor predictions for some of the molecules considered. Since, the viscosity values available at the maximum and minimum temperatures were used for model development as a substitute for the viscosities at the triple point and critical point actually required by the SVRC model, a study was conducted to investigate the effect of variation in the temperature range employed on the model parameters. A random sample set of four compounds (2-methylhexane, dodecane, tridecane, and tetradecane) was used for this study. The results presented in Table A.3 of Appendix A suggest that small changes in the reduced temperature (about 0.01 to 0.05) lead to significant change in the value of the SVRC model parameter. This prompted an additional study on the effect of variations in the parameter α on viscosity predictions. As indicated in Table A.4 of Appendix A, the viscosity predictions show a relatively weak sensitivity to the SVRC parameter values; specifically, errors ranging from -75% to + 75% in the model parameter α resulted in predictions within 10% AAD. Although these deviations show a ten-fold increase in error, the quality of the predictions is comparable to those of the literature models.

Figure 2.4 shows the percentage deviations in liquid viscosities obtained from data regressions using the SVRC model. The figure indicates that most of the data points fall within the ± 2% error bar. The prediction results for the liquid viscosities are depicted in Figures 2.5-2.6. Figure 2.5 shows the percentage distribution of errors in the predicted liquid viscosities. On average, the SVRC model was capable of representing the liquid viscosities within 0.7% AAD, and the generalized SVRC-QSPR model was capable of predicting the liquid viscosities with 1.7% AAD using end-point input data. From Figure 2.5, it is evident that the generalized SVRC-QSPR model predicts the liquid viscosities of the majority of the data points with an AAD of less than 2% using end-point input data. Figure 2.6 presents the percentage deviations in liquid viscosities for the training and the prediction sets as function of the reduced temperature. Overall, five molecules had large prediction errors (AAD greater than 5%). These include (a) 1-hexanol (6.8% AAD), (b) 1-

pentanol, 2-methyl (13.7% AAD), (c) 2-pentanol, 4-methyl (9.6% AAD), (d) 1-octanol (6.3% AAD), and (e) octadecanoic acid (10.2% AAD).

To further validate the predictive capability of the SVRC-QSPR model, an external data set from the DIPPR database that was not included in the model development was used. The external dataset comprised of 15,794 data points involving 622 fluids. Information regarding the molecules used for model validation can be found in Table A2 of Appendix A. This dataset differed from the one that was used for model development in that it contained primarily liquid viscosity values that were obtained from other predictive models and smoothing functions (as reported in the DIPPR database) and was not screened for quality based on reported errors. The limited experimental data contained in this database did not meet the screen criteria of the primary database used for model development. The external dataset contained 47 classes of compounds of which 27 had representation in the training set used in model development. The SVRC-QSPR model was applied to the external dataset. Tables 2.5 and 2.6 present the quality of predictions obtained for the different classes of compounds. Overall, the generalized SVRC-QSPR model was capable of predicting the liquid viscosities of the fluids considered in the external dataset with an AAD of 23%. The temperature ranges and AADs for individual molecules used in the model development can be found in Table A2 of Appendix A. Although the secondary validation process provides valuable insights regarding the predictive ability of the developed generalized SVRC-QSPR model, only a guarded judgment can be made based on this study since the liquid viscosity values reported in the external dataset mostly come from other predictive models and smoothing functions with relatively high reported errors.

The primary goal of this study was to develop a generalized liquid viscosity model capable of providing accurate *a priori* predictions (a) over a wide temperature range in the saturation region, and (b) for a diverse set of molecules involving various functional groups. The SVRC model provides good liquid viscosity representations (AAD of 0.7% for 78 molecules) and predictions by the SVRC-QSPR model (AAD of 1.7%) in comparison to other recommended literature models which, in general, have correlative/predictive capabilities of 5-15 % AAD [5, 6].

The SVRC-QSPR viscosity predictions for a sample of the non-polar fluids were compared to comparable predictions by the recommended literature model [5]. The two models were applied to five heavy alkanes used in the model development because these fluids are deemed to be suitable candidates for the literature model. A favorable comparison is indicated for the SVRC-QSPR model, as indicated by the results shown in Table A.5 of Appendix A.

As evidenced by the results, the generalized SVRC-QSPR model is capable of correlating/predicting the liquid viscosities of a diverse set of molecules with varying structural complexities. Also, our work attempts to model viscosities over a wide temperature as opposed to the currently available QSPR models for liquid viscosities which are restricted to single temperature (298 K) predictions [13-15].

This study was motivated by the fact that neither theory-based models nor neural network based QSPR models alone could provide satisfactory liquid viscosity predictions for diverse chemical compounds. Hence, we hypothesized that an approach, which calls for the use of theory to develop the behavior model, and QSPR to generalize the parameters of such model, is more effective. The quality of the liquid viscosity predictions obtained for such a diverse group of molecules (30 classes involving 1345 data points) demonstrates the validity of this integrated approach and provides credible evidence to support the above hypothesis.

Conclusions

1. The SVRC framework successfully correlated liquid viscosities of a diverse subset of organic molecules over a wide temperature range in the saturation region. The SVRC model was able to represent liquid viscosities of 78 molecules with an AAD of 0.7% on average when one regressed parameter was used for each substance.
2. The SVRC-QSPR model provide reasonable generalized predictions of liquid viscosities, with average errors of less than 1.7%, based on structural descriptors and end-point input data.
3. The generalized model was capable of making *a priori* predictions for an external database of 622 compounds with average errors less than 23%.
4. The results of this study indicate that the use of theory-framed structure-property modeling is effective in thermo-physical model generalization.
5. The limited database employed in the present work constrained the model generalization efforts. These results, however, constitute a promising initial effort in our quest to develop a robust and effective model based on a larger database.

Recommendations

1. Prompt the acquisition of reliable experimental data for liquid viscosities closer to the critical point to determine a precise value for the SVRC critical exponent.
2. Assemble a larger database of experimental measurements involving more diverse molecular species over a wider range of temperature. Availability of such data would facilitate better training of the neural network, which, in turn would lead to the development of a more robust model capable of being extensively validated.
3. Develop a generalized QSPR model for the liquid viscosity at the triple point and the critical point temperatures to serve as input data for the generalized SVRC-QSPR model.
4. Extend the viscosity model to single-phase liquids in general.

References

1. Modern Approaches to Viscosity Measurement, News Release from Hydramotion, *http://www.engineeringtalk.com/news/hdr/hdr113.html*, February 2006.

2. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Vapor Pressures. Fluid Phase Equilibria, 1991. 64: p. 141-163.

3. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Liquid Density. Fluid Phase Equilibria, 1992. 64: p. 81-98.

4. Godavarthy, S., R.L. Robinson, Jr., and K.A.M. Gasem, SVRC-QSPR Model for Predicting Saturated Vapor Pressures of Pure Fluids. Fluid Phase Equilibria, Volume 246, Issues 1-2, 25 August 2006, Pages 39-51.

5. Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Gases and Liquids. 4 ed. 1987: McGraw Hill.

6. Monnery, W.D., W.Y. Svrcek, and A.K. Mehrotra, Viscosity: A Critical Review of Practical Predictive and Correlative Methods. Can. J. Chem. Eng., 1995. 73(February): p. 3.

7. Qun-Fang, L., H. Yu-Chun, and L. Rui-Sen, Correlation of Viscosities of Pure Liquids in a Wide Temperature Range. Fluid Phase Equilibria, 1997. 40: p. 221-231.

8. Martins, R.J., M.J.E.de.M. Cardoso, and O.E. Barcia, A new model for calculating the viscosity of pure liquids at high pressures. Ind. Eng. Chem. Res., 2003. 42: p. 3824-3830.

9. Monnery, W.D., A.K. Mehrotra, and W.Y. Svrcek, Viscosity Prediction of Non-polar, Polar, and Associating Fluids over a Wide Pρt Range from a Modified Square Well Intermolecular Potential Model. Ind. Eng. Chem. Res., 1998. 37: p. 652-659.

10. Quiñones-Cisneros, S.E., C.K. Zéberg-Mikkelsen, and E.H. Stenby, One Parameter Friction Theory Models for Viscosity. Fluid Phase Equilibria, 2001. 178: p. 1-16.

11. Scalabrin, G., G. Cristofoli, and M. Grigiante, A Corresponding States Predictive Viscosity Model Based on a New Scaling Parameter: Application To Hydrocarbons, Halocarbons And Mixtures. International Journal of Energy Research, 2002. 26: p. 1-26.

12. Cruz-Reyes, G., et al., Simultaneous Correlation of Saturated Viscosities of Pure Gases and Liquids Using the Significant Structure Theory. Ind. Eng. Chem. Res., 2005. 44: p. 1960-1966.

13. Suzuki, K., Ohtaguchi, and Koide, Computer-assisted approach to develop a new prediction method of liquid viscosity of organic compounds. Computers Chem. Engng, 1996. 20(2): p. 161-173.

14. Suzuki, T., R.-U. Ebert, and G. Schuurmann, Development of Both Linear and Nonlinear Methods to Predict the Liquid Viscosity at 20°C of Organic Compounds. J. Chem. Inf. Comput. Sci, 1997. 37: p. 1122-1128.

15. Katritzky, A.R., et al., Prediction of Liquid Viscosity for Organic Compounds by a Quantitative Structure-Property Relationship. Journal Of Physical Organic Chemistry, 2000. 13: p. 80-86.

16. S. S. Godavarthy, Design of Improved Solvents for Extractive Distillation, Oklahoma State University, Ph.D. Dissertation, 2004.

17. Project 801, Physical and Thermodynamic Property Database. 1999, Design Institute for Physical Property Data.

18. ChemDraw 8.0. 2004, Cambridge Software.

19. AMPAC 6.0. 1997, Semichem Inc.

20. CODESSA 2.63. 1998, Semichem Inc.

21. Yaffe, D.L., A Neural Network Approach for Estimating Physicochemical Properties Using Quantitative Structure-Property Relationships (QSPRs), University of California: Los Angeles, Ph.D. Thesis, 2001.

22. Ravindranath, D., Structure-Based Generalized Models for Pure-Fluid Saturation Properties and Activity Coefficients, Oklahoma State University: Stillwater, M.S. Thesis, 2005.

23. Mitchell, B. and C.P. Jurs, Prediction of Autoignition Temperatures of Organic Compounds from Molecular Structure. J. Chem. Inf. Comput. Sci, 1997. 37: p. 538-547.

24. Wessel, M.D., J.M. Sutter, and C.P. Jurs, Prediction of Reduced Ion Mobility Constants of Organic Compounds from Molecular Structure. Anal. Chem, 1996. 68: p. 4237-4243.

25. Venkatasubramanian, V., K. Chan, and J.M. Caruthers, Computer-Aided Molecular Design Using Genetic Algorithms. Computers Chem. Engng, 1994. 18(9): p. 833-844.

26. Mitchell, B. and C.P. Jurs, Prediction of Infinite Dilution Activity Coefficients of Organic Compounds in Aqueous Solution from Molecular Structure. J. Chem. Inf. Comput. Sci., 1998. 38: p. 200-209.

27. Wessel, M.D., et al., Prediction of Human Intestinal Absorption of Drug Compounds from Molecular Structure. Molecular Modeling and Prediction of Bioavailability, 2000: p. 249-255.

28. Randic, M., Orthogonal Molecular Descriptors. New J. Chem, 1991. 15: p. 517-525.

29. Lucic, B., et al., The Structure-Property Models Can be Improved Using the Orthogonalized Descriptors. J. Chem. Inf Comput. Sci., 1995. 35: p. 532-538.

30. NeuralWare, Predict 3.10. Feb 2003: Carnegie, PA15106-2700.

31. Sengers, J.V. Transport Properties of Fluids Near Critical Points. in Critical Phenomena. 1970. Villa Monestro: Academic Pres Inc. (London) Ltd.

32. Jagannathan, K. and A. Yethiraj, Moleucular Dynamics Simulations of a Fluid Near its Critical Point. Physical Review Letters, 2004. 93(1): p. 015701-1 to 015701-4.

33. Ohta, T., Multiplicative Renormalization of the Anomalous Shear Viscosity in Classical Liquids. J. Phys. C: Solid State Physics, 1977. 10: p. 791-793.

34. Bhattacharjee, K.J. and A.R. Ferrell, Critical Viscosity Exponent of a Classical Fluid. Physical Review A, 1983. 28(4): p. 2363-2369.

35. Berg, R.F. and M.R. Moldover, Critical Exponent of the Viscosity of Carbon Dioxide and Xenon. J. Chem. Phys, 1990. 93(3): p. 1926-1938.

36. Stanley, E.H., Introduction to Phase Transitions and Critical Phenomena. The International Series of Monographs on Physics, ed. W. Marshall and D.H. Wilkinson. 1971, Oxford and New York: Oxford University Press.

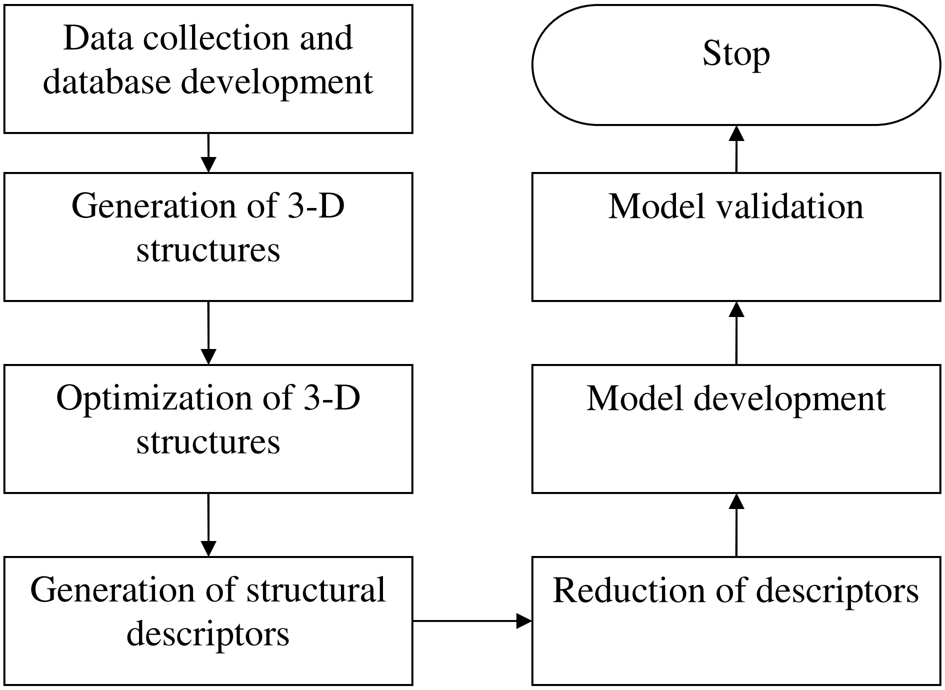

Figure 2.1. Overview of QSPR methodology [16]

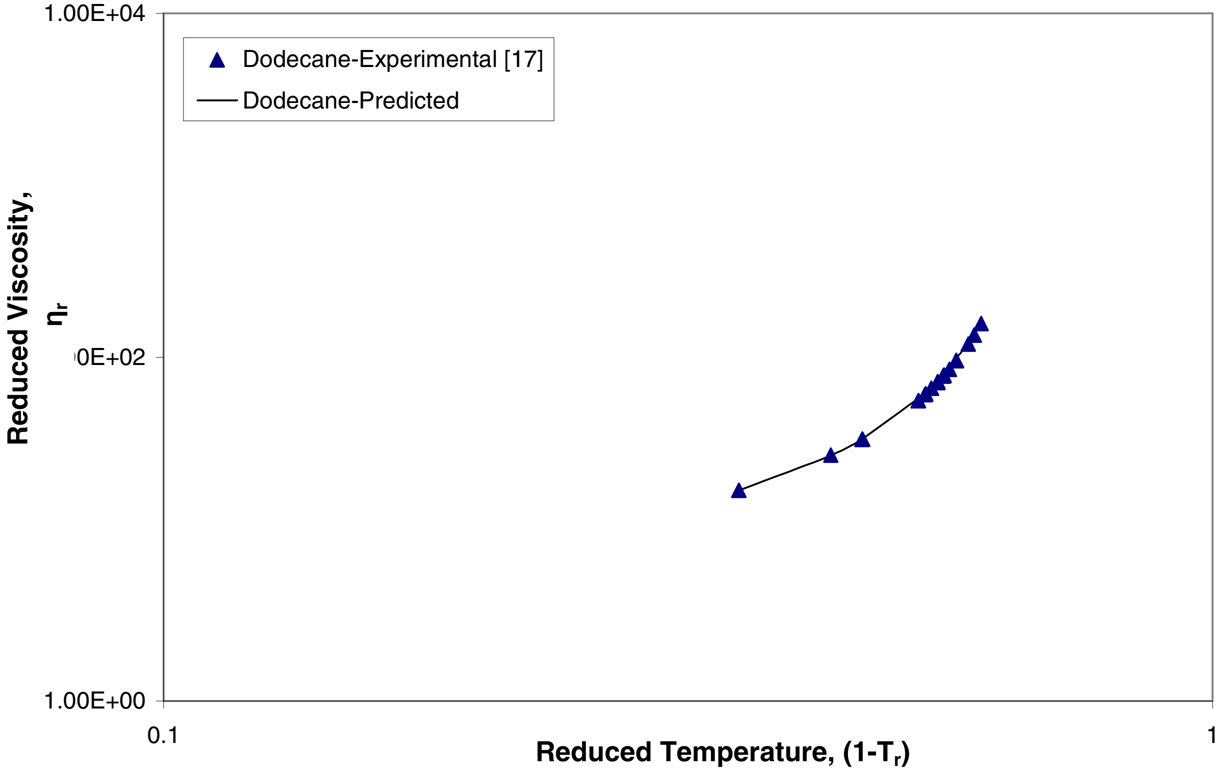

Figure 2.2. Variation of reduced liquid viscosity with temperature

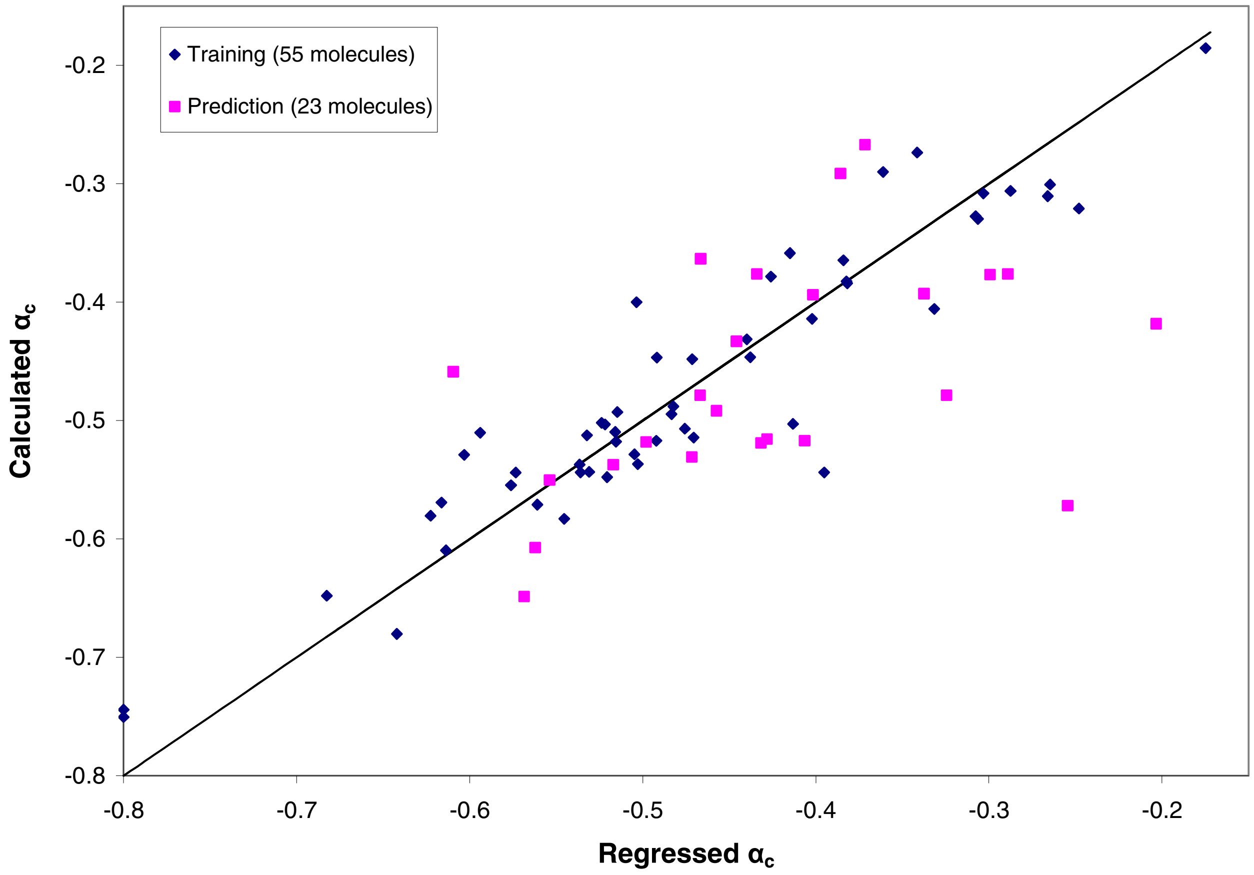

Figure 2.3. Comparison of regressed α_c and calculated α_c of the SVRC-QSPR model for liquid viscosity

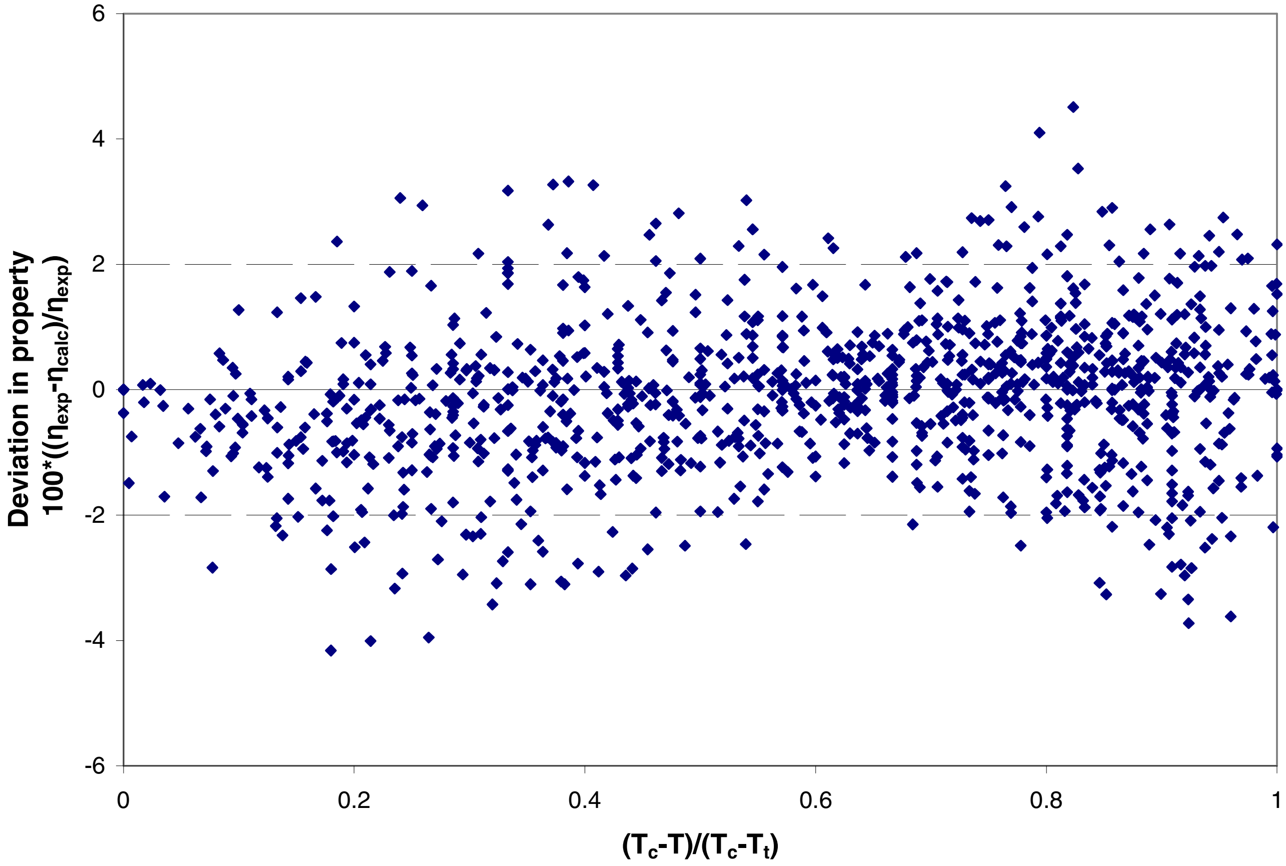

Figure 2.4. Deviations in regressed liquid viscosities using the SVRC model

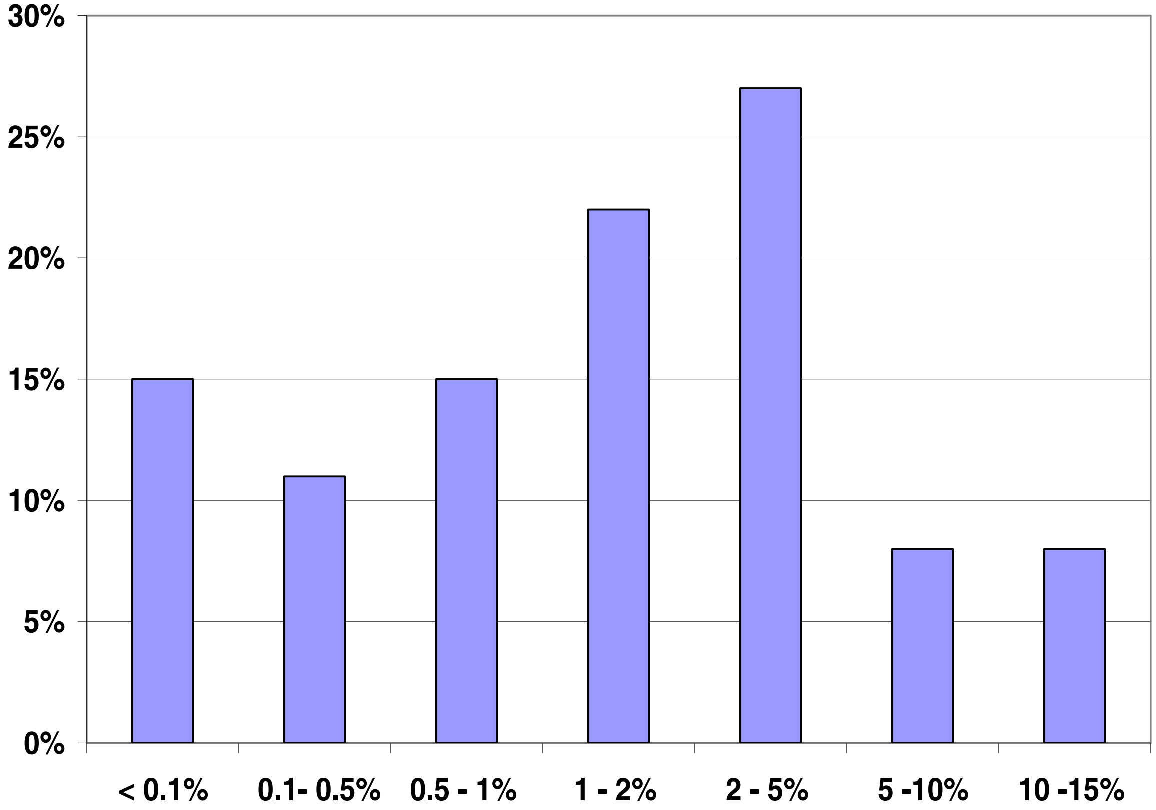

Figure 2.5. Distribution of errors (deviations) in predicted liquid viscosities using the generalized SVRC-QSPR model

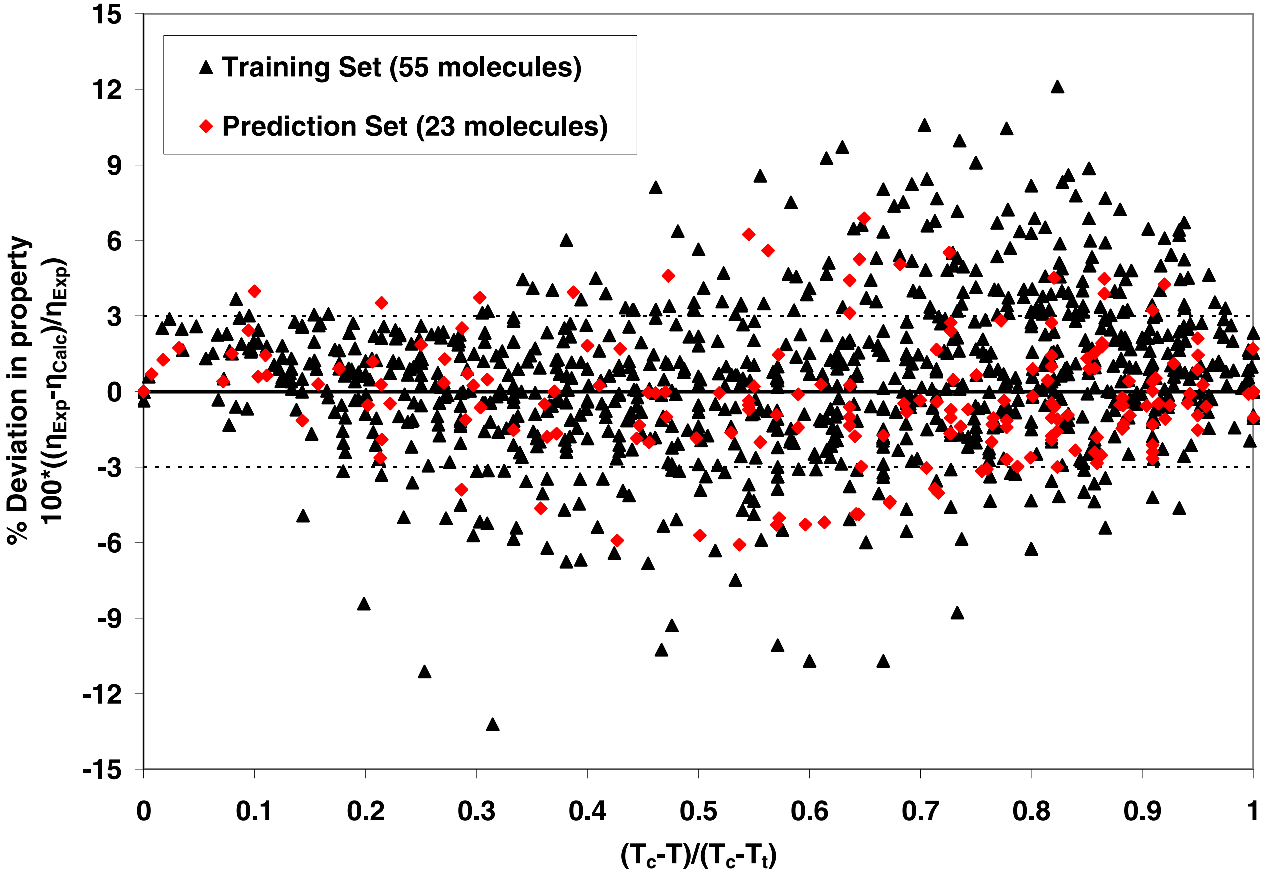

Figure 2.6. Deviations in predicted liquid viscosities using the generalized SVRC-QSPR model.

Table 2.1. Predicted critical exponents characterizing the asymptotic temperature dependence for shear viscosity (η)

Investigator	η (varies as)	y	Basis	Year	Remarks	Reference
Fixman, Deutch, Mountain	ε^{-y}	0.5	Mean Field Theory	1962-67		[30]
Zwanzig	finite		Mean Field Theory	1967-68		[30]
Kadanoff and Swift	ε^{y}	$(\nu-\gamma+\alpha)/2$	Scaling Theory	1968-69	The value of the scaling exponent is 0.245	[30]
Kawasaki	ε^{-y}	0.5	Mean Field Theory	1969		[30]
De Sobrino	ln ε		Mean Field Theory	1969		[30]
Kawasaki	ln ε or finite		Scaling Theory	1970		[30]
Ferrell	ln ε or finite		Scaling Theory	1970		[30]
Halperin and Hohenberg	ε^{-y}	0.043	Renormalization Group Theory		Since, $\xi \sim \varepsilon^{-\nu}$, where, $\nu = 0.63$	[31]
Ohta	ε^{-y}	0.031	Experimental	1977	Values calculated for the following fluids: Xenon and Ethane	[32]
Bhattacharjee and Ferrell	ε^{-y}	0.051	Mode-Coupling Theory	1983		[33]
Bhattacharjee and Ferrell	ε^{-y}	0.042	Mode-Coupling Theory	1986	Since, $\xi \sim \varepsilon^{-\nu}$, Where, $\nu = 0.63$	[33]

Table 2.1. Predicted critical exponents characterizing the asymptotic temperature dependence for shear viscosity (η) (contd.)

Investigator	η (varies as)	y	Basis	Year	Remarks	Reference
Berg and Moldover	ε^{-y}	0.041	Experimental	1990	Values calculated for carbon dioxide and xenon	[34]
Berg, Moldover, and Zimmerli	ε^{-y}	0.043	Experimental	1999	Values calculated for xenon	[31]
Jagannathan and Yethiraj	ε^{-y}	0.043	Molecular Dynamics Simulations	2004	Since, $\xi \sim \varepsilon^{-\nu}$, where, $\nu = 0.63$	[32]

* ε is the symbol used for reduced temperature measured from the critical temperature T_c and is given by $\varepsilon = |T-T_c| / T_c$ and ν, γ, and α are critical exponents of d=3 Ising model (fluid) with values of 0.638, 5/4, and 1/8 respectively [35].

Table 2.2. Summary of results obtained using regressed and predicted SVRC parameters

Compound Name	Case-1 SVRC Regressed Model (% AAD)	Case-2 SVRC-QSPR Model (% AAD)	Reduced Temperature Range (T_r)	Data points
3-METHYLPENTANE	0.5	0.5	0.53-0.66	11
2-METHYLHEXANE	0.3	0.4	0.52-0.69	25
DODECANE	0.3	1.7	0.40-0.65	24
TRIDECANE	0.5	1.1	0.40-0.70	16
TETRADECANE	0.3	1.6	0.40-0.61	23
HEXADECANE	0.9	0.9	0.41-0.78	10
HEPTADECANE	1.1	2.7	0.40-0.78	11
METHYLCYCLOPENTANE	0.2	1.0	0.47-0.66	30
ETHYLCYCLOPENTANE	0.3	0.3	0.44-0.66	28
BUTYLCYCLOHEXANE	0.8	0.8	0.38-0.57	8
CIS-DECALIN	1.5	3.2	0.35-0.64	27
TRANS-DECALIN	0.9	1.8	0.35-0.66	20
1-DECENE	1.1	2.2	0.44-0.67	22
1-HEXADECENE	0.4	0.4	0.38-0.52	9
BENZENE, 1,3-DIMETHYL-	0.5	0.7	0.44-0.58	12
BENZENE, BUTYL	1.1	1.1	0.42-0.55	13
BENZENE, DECYL	1.1	1.3	0.34-0.56	31
BIPHENYL	0.6	0.8	0.45-0.94	27
1,1':4', 1"-TERPHENYL	1.1	2.0	0.53-0.80	22
BENZENE, PENTYL	0.9	1.0	0.42-0.55	11
BENZENE, HEXYL	1.7	3.0	0.36-0.61	24
BENZENE, NONYL	1.2	1.7	0.34-0.54	25
BENZENE, TETRADECYL	0.3	0.5	0.35-0.47	10
BENZENE, ETHENYL	0.4	1.3	0.43-0.66	17
NAPHTHALENE, 1-METHYL-	1.0	1.1	0.35-0.48	9

Table 2.2. Summary of results obtained using regressed and predicted SVRC parameters (contd.)

Compound Name	Case-1 SVRC Regressed Model (% AAD)	Case-2 SVRC-QSPR Model (% AAD)	Reduced Temperature Range (T_r)	Data points
NAPHTHALENE, 2-METHYL-	0.6	0.9	0.41-0.49	18
BENZALDEHYDE, 2-HYDROXY-	0.2	0.2	0.44-0.69	16
TRIOXANE,2,4,6-TRIMETHYL	0.9	1.2	0.49-0.67	13
2-BUTANONE	1.1	1.1	0.42-0.66	13
3-PENTANONE	0.3	0.3	0.49-0.66	19
2-PENTANONE	1.1	1.1	0.49-0.66	26
2-PYROLIDINONE	1.0	1.2	0.37-0.46	14
CYCLOPENTANONE	0.8	1.1	0.47-0.58	18
ETHANONE, 1-PHENYL-	0.5	0.5	0.42-0.52	19
1-HEXANOL	1.6	6.8	0.46-0.70	16
2-HEXANOL	2.1	2.1	0.48-0.70	13
1-PENTANOL, 2-METHYL-	2.8	13.7	0.46-0.68	15
1-BUTANOL, 3-METHYL-	1.7	3.8	0.47-0.70	19
1-HEPTANOL	1.0	1.9	0.46-0.71	8
2-PENTANOL, 4-METHYL-	2.0	9.6	0.49-0.69	15
1-OCTANOL	0.8	6.3	0.44-0.56	14
1-HEXADECANOL	2.4	2.9	0.42-0.74	14
CYCLOHEXANOL	0.3	3.9	0.46-0.66	8
2-PROPEN-1-OL	0.8	0.9	0.52-0.68	19
1,2-BENZENEDIOL	0.7	2.8	0.50-0.66	13
FORMIC ACID	0.4	0.7	0.48-0.64	18
PROPANOIC ACID	0.5	0.8	0.47-0.60	18
PROPANOIC ACID, 2-METHYL-	0.6	1.4	0.45-0.70	34
HEXANOIC ACID	0.6	0.7	0.44-0.56	27
DODECANOIC ACID	1.0	1.0	0.44-0.58	10
OCTADECANOIC ACID	0.6	10.2	0.43-0.59	9

Table 2.2. Summary of results obtained using regressed and predicted SVRC parameters (contd.)

Compound Name	Case-1 SVRC Regressed Model (% AAD)	Case-2 SVRC-QSPR Model (% AAD)	Reduced Temperature Range (T_r)	Data points
ACETIC ACID, ANHYDRIDE	0.3	0.4	0.45-0.67	19
PROPANOIC ACID, ANHYDRIDE	0.5	0.5	0.44-0.70	24
FORMIC ACID, PROPYL ESTER	0.5	0.5	0.51-0.66	18
ACETIC ACID, METHYL ESTER	0.6	0.6	0.54-0.82	38
ACETIC ACID, BUTYL ESTER	0.7	0.7	0.50-0.60	21
1-BUTANOL, 3-METHYL-	0.7	0.9	0.48-0.79	13
PROPANOIC ACID	0.8	0.8	0.51-0.66	20
PROPANOIC ACID, 2-METHYL-	0.4	0.8	0.50-0.67	13
BUTANOIC ACID, ETHYL ESTER	0.7	0.7	0.51-0.60	11
BENZOIC ACID,2-HYDROXY,METHYL ESTER	0.4	0.7	0.42-0.70	6
BENZOIC ACID, ETHYL ESTER	1.3	1.4	0.41-0.49	12
CARBONIC ACID, DIETHYL ESTER	1.4	1.8	0.49-0.68	22
ETHANEDIOIC ACID, DIETHYL ESTER	0.7	1.1	0.44-0.70	13
PROPANEDIOIC ACID, DIETHYL ESTER	1.0	1.0	0.44-0.46	11
PROPANE, 1-ETHOXY-	0.1	0.2	0.55-0.67	12
1,4-DIOXANE	0.5	0.5	0.49-0.64	20
PROPANE, 1,1'-OXYBIS-	0.5	3.0	0.29-0.68	15
ETHANE, 1,2-DIMETHOXY-	1.3	1.3	0.38-0.56	9
BENZENE, ETHOXY-	1.1	1.1	0.42-0.69	22
FURAN, TETRAHYDRO-	0.4	0.7	0.38-0.64	25
2-FURANMETHANOL	0.6	0.8	0.47-0.64	8
ETHANE,2DIFLUOROMETHOXYTRIFLUORO	0.4	0.4	0.56-0.75	20
BENZENE, 1-CHLORO-3-NITRO-	0.4	0.7	0.43-0.57	18
BENZENEACETONITRILE	0.6	0.6	0.40-0.65	10

Table 2.2. Summary of results obtained using regressed and predicted SVRC parameters (contd.)

Compound Name	Case-1 SVRC Regressed Model (% AAD)	Case-2 SVRC-QSPR Model (% AAD)	Reduced Temperature Range (T_r)	Data points
1,2-ETHANEDIOL, NITRATE	0.4	0.4	0.43-0.51	12
PHENOL, 2-METHOXY-	0.6	2.6	0.46-0.69	13
ACETALDEHYDE, TRICHLORO-	0.2	0.2	0.52-0.66	12
Overall % AAD	**0.7**	**1.7**		

Table 2.3. Descriptors obtained from non-linear modeling of SVRC liquid viscosity model parameter α_c

Descriptors
Molecular weight
Min e-n attraction for a C-H bond
PPSA-3 Atomic charge weighted PPSA [Quantum-Chemical PC]
Max electroph. react. index for a C atom
Min nucleoph. react. index for a O atom
ZX Shadow / ZX Rectangle
Randic index (order 3)
Number of O atoms

Table 2.5. Results of secondary validation for the generalized SVRC-QSPR model using an external dataset

Chemical Classes Represented in the Training Set	%AAD	Datasets
1-ALKENES	22.5	17
ALKYLCYCLOPENTANES	12.2	11
ANHYDRIDES	10.1	8
AROMATIC ESTERS	22.7	3
CYCLOALIPHATIC ALCOHOLS	45.9	5
DIPHENYL/POLYAROMATICS	8.6	16
KETONES	6.4	33
METHYLALKANES	16.2	17
MULTIRING CYCLOALKANES	1.2	3
N-ALCOHOLS	42.4	20
N-ALIPHATIC ACIDS	6.3	14
N-ALKANES	26.7	28
N-ALKYLBENZENES	33.0	14
OTHER ALIPHATIC ACIDS	7.8	12
OTHER ALIPHATIC ALCOHOLS	31.1	29
OTHER ALKYLBENZENES	13.9	39
OTHER ETHERS/DIETHERS	5.6	2
OTHER MONOAROMATICS	7.3	18
OTHER POLYFUNCTIONAL C, H, O	1.6	3
OTHER SATURATED ALIPHATIC ESTERS	19.1	7
POLYFUNCTIONAL C, H, O, N	12.9	2
POLYOLS	28.5	30
PROPIONATES AND BUTYRATES	5.0	9
2,3,4-ALKENES	6.3	18
ACETATES	8.4	12
ALDEHYDES	2.9	28
ALKYLCYCLOHEXANES	7.7	17

Table 2.6. Results of secondary validation for the generalized SVRC-QSPR model using an external dataset

Chemical Classes not Represented in the Training Set	%AAD	Datasets
ALKYNES	4.5	17
AROMATIC ALCOHOLS	19.4	16
AROMATIC CARBOXYLIC ACIDS	3.5	4
CYCLOALKANES	5.2	6
CYCLOALKENES	12.8	7
DIALKENES	3.7	23
DICARBOXYLIC ACIDS	2.3	3
DIMETHYLALKANES	10.3	16
ELEMENTS	18.1	4
ETHYL & HIGHER ALKENES	15.5	12
FORMATES	3.9	10
INORGANIC GASES	19.3	8
METHYLALKENES	11.7	16
NAPHTHALENES	11.1	15
OTHER ALKANES	20.9	23
OTHER CONDENSED RINGS	7.9	8
OTHER HYDROCARBON RINGS	12.5	3
POLYFUNCTIONAL ACIDS	4.0	2
TERPENES	11.9	8
UNSATURATED ALIPHATIC ESTERS	4.2	6

CHAPTER 3

SVRC-QSPR MODEL FOR VAPOR VISCOSITIES

Introduction

Viscosity is an important transport property used in engineering design for transportation and processing of fluids. Techniques for measuring the viscosity of fluid samples have been available in abundance for many years. Despite their widespread use, however, many of them are time-consuming, expensive, and unreliable. Operational and maintenance problems plague the process of making experimental viscosity measurements [1]. These problems are further amplified in the case of hazardous chemicals where handling and storage cause a problem. Although conducting experimental measurements is still the preferred method for determining the desired properties, reliable models capable of providing a *priori* predictions would certainly supplement the process, especially when dealing with new and challenging chemicals. The correlations available in the literature for predicting vapor viscosity currently have a limited range of applicability or poor suitability for generalization. Further, most of the literature models exhibit large errors near the critical point of the fluid and rely on experimentally measured physical properties as input for their predictions.

Generalizations made using these traditional physical properties do not capture the subtleties of various chemical structures and hence provide poor predictions. Moreover, the values for these physical properties are not available for numerous new and structurally complex molecules. Quantitative structure-property relationship (QSPR) models offer an attractive alternative since they have the potential to provide reliable property estimates based on chemical structure information alone. Literature studies which use structural descriptors for correlation of liquid viscosities have been published. However, currently available QSPR models for liquid viscosity are limited to predictions at a single temperature and/or are restricted to a narrow range of chemical species. Also, most of these models use experimentally determined physical properties as descriptors and hence are restricted only for those compounds for which these data are available.

Previously, researchers at Oklahoma State University (OSU) have developed a unified framework for correlating saturation properties, which include vapor pressure, liquid and vapor densities [2, 3]. This scaled-variable-reduced-coordinates (SVRC) model is based on the corresponding states theory (CST) and scaling-law behavior, and, in general, it is capable of representing saturation properties within their experimental uncertainties. In this work, we attempt to extend the SVRC model to correlate saturated vapor viscosities and generalize the model parameters using structure-property modeling. A database of 438 data points involving 29 fluids was used to develop this model and an external dataset containing 4746 data points involving 475 fluids was used for secondary validation of the model. The approach involves the use of QSPR methodology to generalize the SVRC model parameters. Specifically, we use the SVRC model to correlate the vapor viscosities, and QSPR to generalize the parameters of such a model. This approach, in the past, has proven to be more effective than the typical efforts to develop generalized models directly using QSPR techniques [see, e.g., 3]

Vapor Viscosity Prediction Models

Vapor phase viscosity is a function of momentum transfer by translation of the molecules with relatively few collisions and is well described by the kinetic theory of gases. The simplest kinetic model for estimating dilute-gas viscosity considers the molecules comprising the gas as non-interacting rigid spheres of diameter σ and mass m moving at some mean velocity and colliding with other such molecules after moving a 'mean free path' distance. The kinetic theory gives the following expression for computing dilute-gas viscosity [5]:

$$\eta_0 = \left(2/3\pi^{3/2}\right)\left[(mkT)^{1/2} / \sigma^2\right] \tag{1}$$

To account for molecular interactions (attraction and repulsion due to intermolecular forces), the Chapman-Enskog (CE) theory is normally applied. The CE theory treats the interaction between the molecules and gives the following equation to compute viscosity [5]:

$$\eta_{CE} = \left(5/16\pi^{1/2}\right)\left[(mkT)^{1/2} / \left(\sigma^2\omega^{2,2}(T^*)\right)\right] \tag{2}$$

The above equation contains the collision integral $\omega^{2,2}(\mathrm{T}^*)$. For hard spheres, the collision integral is set to be unity. Otherwise, the collision integral is said to be a function of dimensionless temperature and depends on the intermolecular potential function chosen. The correlation for collision integral defined for Lennard-Jones intermolecular potential is given by [5]:

$$\omega = A(T^*)^{-B} + Ce^{(-DT^*)} + Ee^{(-FT^*)} \tag{3}$$

where, A = 1.16145, B = 0.14874, C = 0.52487, D = 0.77320, E = 2.16178 and F = 2.43787 [5]. The CE theory deals only with spherically symmetric mono-atomic molecules with no internal degrees of freedom. Owing to the complexity in describing the dynamics of collisions among the molecules, simple empirical correlations have been used for practical purposes [5]. A review of the most commonly used correlative and predictive methods to estimate vapor viscosity has been done by Reid and co-workers [6] and Monnery and co-workers [5]. A brief summary of efforts by authors in recent times is summarized in the following paragraph.

Zhang and co-workers [7] developed a correlation employing the thermo-physical properties: critical temperature, critical pressure, critical specific volume, molecular weight and acentric factor to predict the viscosity of halides within 5% of the measured values. Shan and co-workers [8] developed a model for calculation of viscosity of trifluoromethane (R-23) expressed in terms of temperature and density. The model is based on Eyring's significant structure theory and is applicable to a wide range of thermodynamic conditions including dilute gas, liquid, saturated vapor, saturated liquid, critical and supercritical regions. The authors claim an estimated accuracy of ±1% for their correlation. Hildwein and Stephen in 2005 developed a viscosity model for pure fluids based on the significant structure theory (SST). The model uses five adjustable parameters that are determined from experimental data. The model has the correlative capability to represent the saturated vapor viscosity in the range of 1.6-6.9% for 14 non-polar and three polar compounds [9]. Reyes and co-workers [9] proposed a viscosity model based on the SST coupled with a cubic equation of state for the simultaneous correlation of viscosities of pure liquids and gases (polar and non-polar) at saturated conditions. The predictive capability of the model was tested on two pure fluids:

water and propane. This model was capable of representing the saturated liquid and vapor viscosities of these compounds with a %AAD of 3.7 and 3.4, respectively.

For practical engineering purposes, models with minimum number of parameters that are amenable to generalization are required.

Scaled-Variable-Reduced-Coordinate Framework

In previous studies [2, 3], the SVRC framework was used to correlate saturation properties of a wide variety of organic molecules over the entire saturation range. The SVRC model utilizes corresponding states theory (CST) and scaling-law behavior.

The general SVRC framework for correlation of thermo-physical properties is given as [1, 2]:

$$\left(Y_\infty^\alpha - Y^\alpha\right)/\left(Y_\infty^\alpha - Y_0^\alpha\right) = \Theta(\varepsilon) \tag{1}$$

Or

$$Y^\alpha = Y_0^\alpha \Theta(\varepsilon) + \left[1 - \Theta(\varepsilon)\right] Y_\infty^\alpha \tag{2}$$

where,

$$\varepsilon = \left(X_\infty - X\right)/\left(X_\infty - X_0\right) \tag{3}$$

$\Theta(\varepsilon)$ is the correlating function, X is the correlating variable, Y is the saturation property at given X, Y_∞ is the asymptotic value of saturation property at X_∞, Y_0 is the initial value of saturation property at X_0 and α is the scaling exponent.

To correlate saturation properties, Equation (1) is recast for representing the various properties between the triple and the critical points as:

$$Y = \left\{ Y_c^{\alpha} - \left(Y_c^{\alpha} - Y_t^{\alpha} \right) \Theta \right\}^{(1/\alpha)} \tag{4}$$

Applied specifically to vapor viscosity, the above equation is written as:

$$\eta = \left\{ \eta_c^{\alpha} - \left(\eta_c^{\alpha} - \eta_t^{\alpha} \right) \Theta \right\}^{(1/\alpha)} \tag{5}$$

where, η_c and η_t are the critical and triple point viscosities, respectively. In this work, due to restricted availability of data, the vapor viscosity data at the lowest and the highest temperatures available were taken to be η_c and η_t for modeling purposes.

The functions $\Theta(\varepsilon)$ and α are defined as:

$$\Theta(\varepsilon) = \frac{\left(1 - A^{\varepsilon^B}\right)}{(1 - A)} \tag{6}$$

$$\alpha = \alpha_c - \mathit{\Delta}\alpha \frac{\varepsilon(1 + C\varepsilon)}{1 + C} \tag{7}$$

where

$$\varepsilon = \frac{T_c - T}{T_c - T_t} \tag{8}$$

and

$$\mathit{\Delta}\alpha = \left(\alpha_c - \alpha_t \right) \tag{9}$$

A, B and C are correlation constants, α_c and α_t are the limiting values of α at the critical temperature and triple point temperature, respectively. The SVRC model accounts for the effects of temperature and chemical structure through the correlating function (Θ) and the scaling function (α). In the current study, the value of $\Delta\alpha$ (in Equation 7) is set to be zero (or $\alpha_c = \alpha_t = \alpha$); thus, a single-parameter model is used.

QSPR Methodology

Computational techniques have gained popularity recently owing to the advances in technology. They are increasingly used to address complex engineering and design problems in chemical processing. The QSPR approach is among the computational methods gaining wide use. It is based on the assumption that there exists a relationship between the structure of a substance and its physical and chemical properties. QSPR uses quantum mechanics to define the structure of the molecule in terms of a series of molecular descriptors and then correlates the property in terms of these descriptors. The following steps are part of any QSPR model development effort [10] (a) generation of 3-D structures, (b) optimization of 3-D structures, (c) calculation of descriptors, (d) reduction of descriptors, and (e) development of a QSPR model. The procedure used to develop QSPR generalization for the SVRC model parameters (α_c, α_t) are outlined in the following paragraphs.

Database Development

A property database of pure fluids including alkanes, refrigerants, aromatics and alcohols was used in the SVRC saturated vapor viscosities model development. The data used in this study were compiled mainly from the DIPPR database [11]. The DIPPR database, on the whole, contained 21,316 vapor viscosity data points involving 1666 fluids. This database was screened to include only organic compounds for which quality experimental data (with reported errors of less than 5%) was available. Also, only datasets with more than six data points were included in the model development procedure. The screened database contained over 459 saturated vapor viscosities data points involving 31 fluids. To the extent possible, for each compound, we sought data that covered a wide temperature range in the saturation region.

Data points with percent absolute average deviation (%AAD) greater than twice the overall regression %AAD of a compound were eliminated from the database in an effort to remove data with large uncertainties. Based on this procedure, a total of 21 data points were eliminated which constituted about 8.4% of the total. The reduced database finally contained 420 data points involving 28 fluids. A list of the compounds used and the reduced temperature ranges for each molecule can be found in Table A.2 of Appendix A. It should be noted that currently, limited experimental data are available in the literature for viscosities. Even when available, they are restricted to a single temperature (298 K) or a narrow temperature range. Particularly, data near the critical point is nearly non-existent. This maybe attributed to the practical difficulties in measuring viscosity near the critical point.

Structure Generation

The first step in any QSPR modeling effort is the generation of chemical structures. Various kinds of chemical representation have been proposed in the literature. The most common way of representing a chemical is a two-dimensional (2-D) sketch [10]. But, the drawback of using a 2-D representation is that it does not provide a complete description of the molecule and cannot be conveniently used for database storage and searching [10]. To have an efficient QSPR model, the representation of a molecule should provide all the necessary structural information. This requires information about the atoms present, along with three-dimensional (3-D) coordinates that provide a full spatial depiction of the molecule. A commercial package, ChemDraw [12] was used to generate the 3-D structures of the molecules.

Structure Optimization

More than one set of 3-D coordinates can be generated for any given molecule. Most molecules contain single bonds that join two groups of atoms. Such bonds can usually rotate with a low-to-moderate energy barrier that changes the orientation of other groups in the structure and thereby the value of the descriptors [10]. In nature, all these representations occur in differing probability and the objective of structure optimization is to obtain a 3-D structure which is most prominent and has the minimal potential energy surface. In this work, the 3-D structures generated were first optimized using the MOPAC routine available in the ChemDraw package and later using commercial optimization software called AMPAC [13]. The use of two optimization routines practically eliminated any un-optimized structures. Intricate details of 3-D structure generation and optimization are beyond the scope of this work. A detailed explanation can be found elsewhere [10, 13].

Descriptor Generation

Once an accurate 3-D structure of a chemical has been obtained, the next step involves calculation of the molecular descriptors. The molecular descriptors calculated by any commercial package are usually divided into (1) constitutional, (2) topological, (3) geometrical, (4) electrostatic, (5) quantum-chemical and (6) thermodynamic. Details about these classes of descriptors can be found elsewhere [10]. In this work, commercial software called CODESSA [14] was used to generate the descriptors. Around 400 descriptors were generated for each molecule. The actual number of descriptors calculated for each molecule varied based on the structural complexity of the molecule.

Descriptor Reduction

All the 400 descriptors generated for each molecule are not significant in modeling vapor viscosities. The use of all available descriptors in the model development effort causes dimensionality problems. Further, the use of irrelevant or redundant descriptors diminishes the performance of a QSPR model, especially when non-linear algorithms are used in model development. Descriptor reduction (DR) is the process of automating the discovery of potentially useful correlations from large sets of descriptor data [10]. The DR process involves the identification of the most relevant set of descriptors for model development and is the most important step in all QSPR model development efforts. Several different methods for DR are available in the literature. The most widely used techniques are the principal-component analysis (PCA), partial least-squares (PLS), genetic algorithms (GA), and neural networks (NNs) [10].

Most QSPR models developed have been based on multiple linear regression correlations requiring *a priori* assumption of the form of the mathematical correlation model. Such models do not consider the non-linearity that may exist among the input parameters and the output properties. The above deficiencies have been addressed in the past using Artificial Neural Networks (ANN). Neural networks are powerful tools for correlating, predicting and classifying large complex data sets. It can successfully deal with non-linearity, handle noisy or irregular data, correlate hundreds of variables or parameters, and provide generalized solutions [15]. However, commonly-used neural network architectures, such as back propagation networks, demand extensive training (using a significant amount of data) to develop a stable QSPR model [16]. This places further demands on modeling efforts since reliable experimental data are not easily available. Another Artificial Intelligence (AI) tool that has been used in

QSPR model development is the Genetic Algorithms (GA) [17, 18]. Genetic search methods are based on Darwinian models of natural selection and evolution. The general idea behind genetic algorithms is the evolutionary creation of a new population of entities from an earlier generation through crossover and mutation processes and by passing on the fittest offspring to the next generation [19]. This approach is ultimately expected to lead to generations that become fitter through evolution thereby achieving the desired objective. More details on GA can be found elsewhere [19].

Hybrid approaches using genetic algorithms and neural networks have also been recently proposed, and have shown good promise in developing accurate and robust QSPR models [20, 21]. In this work, such a hybrid approach employing Genetic Algorithms and Neural Networks was used to develop a generalized non-linear model for vapor viscosities.

QSPR Model Development

This work aimed at (a) demonstrating the ability of the SVRC model to precisely represent saturated vapor viscosities using one regressed parameter, (b) examining the efficacy of using QSPR algorithms to obtain estimates for the SVRC parameter based on chemical structure information using non-linear algorithms. Two case studies were conducted in sequence to achieve these objectives:

Case 1. Determination of the SVRC parameter (α) by regressing experimental data

Case 2. Generalization of the SVRC parameter using non-linear structure-based models

The vapor viscosity model development was initiated with the regression of the SVRC parameter for each molecule (Case 1). As can be seen from Equations 5-7, the SVRC model for vapor viscosity has five parameters A, B, C, α_c, and α_t. Since the value of $\Delta\alpha$ is set to zero,

α_c becomes equal to α_t and the model is reduced to a one-parameter (α) model. Amongst these, A, and C are treated as universal constants applicable to all fluids. Based on regression, the values of these constants are fixed to be the following: A=1.33; C=0. B is the universal scaling exponent, which characterizes the divergence of viscosity near the critical point. Several values for this exponent have been proposed in the literature. A comparative study of these values is presented in Table 3.1. But, when the exponent values suggested in the literature were used for fitting the available experimental data, large errors were obtained. So, based on subsequent regressions, a value of 1.0 for B was used with the two universal constants (A=1.33; C=0), and one adjustable parameters ($\alpha_c = \alpha$). As shown in Figure 3.2, this combination of constants provided good representation of the data. The lack of experimental viscosity data close to the critical point precluded us from determining a precise value for the critical exponent B that is reconcilable with the values proposed in the literature. The parameter α is treated as substance specific. A rigorous generalization strategy based on chemical structure information alone was adopted.

Structure-based model development was initiated with structure generation, optimization, and descriptor generation. Studies have shown that structural descriptors are often highly correlated leading to numerical instabilities commonly referred to as multicollinearity. In such instances, it becomes increasingly difficult to disentangle the unique effects of each predictor (descriptor) on the response variable. Multicollinearity results in highly unstable estimated regression coefficients, the values of which are extremely sensitive to addition/removal of variables or small changes in data points leading to erroneous results and interpretations [22]. To tackle this problem, the use of orthogonal molecular descriptors was suggested. The procedure of orthogonalization focuses on the residuals of intercorrelation between descriptors thereby ensuring that distinct structural characteristics of various descriptors are extracted and used as novel descriptors, which are free from mutual relatedness [22]. More information on the procedure of orthogonalization and its use can be found elsewhere [22, 23]. In this work, the descriptors generated by CODESSA were orthogonalized to obtain a subset of descriptors from which all redundant information has been removed. Non-linear DR techniques were then applied to this reduced subset of descriptors.

The non-linear modeling was performed using commercial software [24]. The reduced subset of descriptors obtained from the orthogonalization step is exported to the software which has a Microsoft Excel™ interface. The software employs GA to identify the best set of input variables for the model. GA operates on a population of individuals. The population changes from one generation to the next, usually by combining characteristics of two "parent" individuals to create a "child" individual. Every individual is assigned fitness and the concept of "survival of the fittest" is implemented by selecting the fit parents more frequently than less fit parents to create the next generation [25].

In this case, an "individual" is actually a set of descriptors. The fitness of a descriptor is derived from the performance of a model that uses the descriptor's variable set as inputs. The algorithm begins with descriptors that consist of small sets of variables. Descriptors that produce good models are kept in the population and used to generate descriptors that consist of larger sets of variables if necessary. In general, however, smaller variable sets (that is, fewer model inputs) are preferred to larger variable sets. The fitness of a descriptor is evaluated using Neural Networks. The software constructs the actual neural network incrementally, using a technique known as cascade correlation. Hidden units are periodically added, usually one or two at a time. Each time a hidden unit or pair of hidden units is added, weights are trained from several different initialization values. Each initialization is referred to as a candidate. The best candidate is established in the network, and then all the weights to the output node(s) of the network are retrained.

There are several heuristics that provide guidance to the permissible number of hidden neurons or choice of networks weights and criteria for termination of training. For example, when determining the network architecture, the rule of thumb is to keep the ratio of total observations (number of molecules) to adjustable parameters (network weights) above two to avoid any chance effects. However, these rules are just for guidance and trial-and-error investigation remains the reliable method for choosing the optimum parameters [4]. To construct the neural network model, the data set containing 28 molecules were randomly split into training and prediction (test) sets. The training and prediction sets contained 70% and 30% of the data, respectively. After rigorous trial-and-error analysis, a neural network was developed for the SVRC model parameter (α). Specifically, a 5-2-1 (5 descriptors - 2 hidden neurons - 1 output variable) architecture was obtained using the training set. The SVRC parameters for the prediction set were then generated using the 5-2-1 network. The efficacy of the neural network model, as indicated by its accuracy and stability, is evaluated based on the quality of the model predictions (overall % AAD) obtained from the SVRC model as given by Equation 5.

Results and Discussion

Table 3.2 presents the summary results for the case studies conducted. The entire data set containing 28 molecules was correlated using a one-parameter SVRC model. As indicated by the results for Case 1, the SVRC model represents the vapor viscosities of the diverse organic subset over a wide temperature range in the saturation region, with AAD of 0.4% using one regressed parameter.

The SVRC parameter (α) was then generalized using non-linear QSPR models (Case 2). A hybrid approach employing Genetic Algorithms and Neural Networks was used to identify the best non-linear model that provided accurate predictions. GA was used to identify the best subset of descriptors and NN was used to evaluate the fitness of the selected individuals (descriptors). A Tan H transfer function [24] was used and several architectures were investigated by varying the number of hidden neurons. A 5-2-1 architecture for the parameter, α, was found to provide the best performance as measured from the overall %AAD of the property predictions from the model. The number of adjustable parameters in the network architectures for both the model parameters was also found to obey the above mentioned heuristic (ratio of number of systems used for training to the number of adjustable parameters being greater than two). The descriptors generated from the non-linear model are presented in Table 3.3.

A comparison plot between the regressed SVRC parameters and the parameters calculated from the non-linear QSPR models is presented in Figure 3.3. The plot shows the efficacy of the neural network model in predicting the parameters. The limited data available for training constrained the model development efforts resulting in poor predictions for some of the molecules considered. Figure 3.4 shows the percentage deviations in vapor viscosities obtained from data regressions using the SVRC model. The figure indicates that most of the data points fall within the ± 2% error bar.

The prediction results for the vapor viscosities are depicted in Figures 3.5-3.6. Figure 3.5 shows the percentage distribution of errors in the predicted vapor viscosities while Figure 3.6 represents the percentage deviations in vapor viscosities for the training and the prediction sets with respect to the reduced temperature. From Figures 3.5 and 3.6, it is evident that the generalized SVRC-QSPR model predicts the vapor viscosities of the majority of the data points with an AAD of 2%. On average, the SVRC model was capable of representing the vapor viscosities with an AAD of 0.4% and the generalized SVRC-QSPR model was capable of predicting the vapor viscosities with an AAD of 0.6% using end-point input data.

To further validate the predictive capability of the SVRC-QSPR model, an external data set from the DIPPR database that was not included in the model development was used. The external dataset comprised of 5707 data points involving 679 fluids. A list of the molecules used for the external validation is provided in Table B.2 of Appendix B. This dataset differed from the one that was used for model development in *that it primarily contained vapor viscosity values that were obtained from other predictive models and smoothing functions* (as reported in the DIPPR database) and was not screened for quality based on reported errors. The limited experimental data contained in this database did not meet the screen criteria of the primary database used for model development. The external dataset contained 47 classes of compounds of which seven had representation in the training set used in model development. The data in the external dataset were culled to separate the classes of compounds that had representation in the training set from the ones that did not. The generalized SVRC-QSPR model was initially applied to fluids belonging to chemical classes which had representation in the training set (1456 data points involving 125 fluids (datasets)).

The predictions obtained from the model were compared to the values reported in the external dataset. In general, the model was capable of predicting the vapor viscosities of fluids belonging to a majority of the chemical classes with an AAD of <5%. Table 3.4 shows the AADs obtained for the different classes of compounds in the external dataset that had representation in the training set. The generalized model was then applied to fluids belonging to chemical classes that did not have representation in the training set (4251 data points involving 554 fluids). The results for the same are presented in Table 3.5. With few exceptions, the results indicate that the classes of compounds that are represented in the training set have lower prediction errors than the ones that do not have representation.

Although the secondary validation process provides valuable insights regarding the predictive ability of the developed generalized SVRC-QSPR model, only a guarded judgment can be made based on this study since the vapor viscosity values reported in the external dataset mostly come from other predictive models and smoothing functions with relatively high reported errors.

The primary goal of this study was to develop a generalized vapor viscosity model capable of providing accurate *a priori* predictions (a) over a wide temperature range in the saturation region, and (b) for a diverse set of molecules involving various functional groups. Our model provides good vapor viscosity representations (AAD of 0.4% for 28 molecules) and predictions (AAD of 0.6%) in comparison to other recommended literature models which, in general, have correlative/predictive capabilities of 5-15 %AAD [5, 6]. The predictions obtained were compared to the models recommended in the literature [5]. The results obtained for selected polar and non-polar compounds are presented in Table B.3 of Appendix B. A favorable comparison is indicated for the SVRC-QSPR model.

As evidenced by the results, the generalized SVRC-QSPR model is capable of correlating/predicting the vapor viscosities of a diverse set of molecules with varying structural complexities.

This study asserts that neither EOS models nor neural network based QSPR models alone could provide satisfactory vapor viscosity predictions for diverse chemical compounds. Hence, we hypothesized that an approach, which calls for the use of theory to develop the behavior model, and QSPR to generalize the parameters of such model, is more effective. The quality of the vapor viscosity predictions obtained for such a diverse group of molecules demonstrates the validity of this integrated approach and provides credible evidence to support the above hypothesis.

Conclusions

1. The SVRC framework successfully correlated vapor viscosities of a diverse subset of organic molecules over a wide temperature range in the saturation region. The SVRC model was able to represent vapor viscosities of 28 molecules with an AAD of 0.4% on average when one adjustable parameter was used for each substance.
2. The SVRC-QSPR model provides reasonable generalized predictions of vapor viscosities, with average errors of less than 0.6%, based on structural descriptors and end-point input data.
3. The generalized model was capable of making *a priori* predictions for an external database of 679 compounds with an overall AAD of 2.7%.
4. The results of this study indicate that the use of theory-framed structure-property modeling is effective in thermo-physical model generalization.

5. The limited database employed in the present work constrained the model generalization efforts. These results, however, constitute a promising initial effort in our quest to develop a robust and effective model based on a larger database.

Recommendations

1. Prompt the acquisition of reliable experimental data for vapor viscosities closer to the critical point to determine a precise value for the SVRC critical exponent.
2. Assemble a larger database of experimental measurements involving more diverse molecular species over a wider range of temperature. Availability of such data would facilitate better training of the neural network, which, in turn, would lead to the development of a more robust model capable of being extensively validated.
3. Develop a generalized QSPR model for the liquid viscosity at the triple point and the critical point temperatures to serve as input data for the generalized SVRC-QSPR model.
4. Extend the viscosity model to single-phase gases in general.

References

1. Modern Approaches to Viscosity Measurement, News Release from Hydramotion, http://www.engineeringtalk.com/news/hdr/hdr113.html, February 2006.

2. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Vapor Pressures. Fluid Phase Equilibria, 1991. 64: p. 141-163.

3. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Liquid Density. Fluid Phase Equilibria, 1992. 64: p. 81-98.

4. Godavarthy, S., R.L. Robinson, Jr., and K.A.M. Gasem, SVRC-QSPR Model for Predicting Saturated Vapor Pressures of Pure Fluids. Fluid Phase Equilibria, Volume 246, Issues 1-2, 25 August 2006, Pages 39-51.

5. Monnery, W.D., W.Y. Svrcek, and A.K. Mehrotra, Viscosity: A Critical Review of Practical Predictive and Correlative Methods. Can. J. Chem. Eng., 1995. 73(February): p. 3.

6. Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Gases and Liquids. 4 ed. 1987: McGraw Hill.

7. Zhang, Z. and Z. Liu, Method for Calculating Viscosity of Halides at Saturated Vapor State. Journal of Xi'an Jiaotong University, 1999. v 33(n 5): p. 42-44.

8. Shan, Z., S.G. Penoncello, and R.T. Jacobsen. Generalized Model for Viscosity and Thermal Conductivity of Trifluoromethane (R-23). in 2000 ASHRAE Winter Meeting. 2000. Dallas, TX, USA: Amer. Soc. Heating, Ref. Air-Conditioning Eng. Inc., Atlanta, GA, USA.

9. Reyes, G.C., et al., Simultaneous Correlation of Saturated Viscosities of Pure Gases and Liquids using the Significant Structure Theory. Ind. Eng. Chem. Res, 2005. 44: p. 1960-1966.

10. S. S. Godavarthy, Design of Improved Solvents for Extractive Distillation, Oklahoma State University, Ph.D. Dissertation, 2004.

11. Project 801, Physical and Thermodynamic Property Database. 1999, Design Institute for Physical Property Data.

12. ChemDraw 8.0. 2004, Cambridge Software.

13. AMPAC 6.0. 1997, Semichem Inc.

14. CODESSA 2.63. 1998, Semichem Inc.

15. Yaffe, D.L., A Neural Network Approach for Estimating Physicochemical Properties Using Quantitative Structure-Property Relationships (QSPRs), University of California: Los Angeles, Ph.D. Thesis, 2001.

16. Ravindranath, D., Structure-Based Generalized Models for Pure-Fluid Saturation Properties and Activity Coefficients, Oklahoma State University: Stillwater, M.S. Thesis, 2005.

17. Mitchell, B. and C.P. Jurs, Prediction of Autoignition Temperatures of Organic Compounds from Molecular Structure. J. Chem. Inf. Comput. Sci, 1997. 37: p. 538-547.

18. Wessel, M.D., J.M. Sutter, and C.P. Jurs, Prediction of Reduced Ion Mobility Constants of Organic Compounds from Molecular Structure. Anal. Chem, 1996. 68: p. 4237-4243.

19. Venkatasubramanian, V., K. Chan, and J.M. Caruthers, Computer-Aided Molecular Design Using Genetic Algorithms. Computers Chem. Engng, 1994. 18(9): p. 833-844.

20. Mitchell, B. and C.P. Jurs, Prediction of Infinite Dilution Activity Coefficients of Organic Compounds in Aqueous Solution from Molecular Structure. J. Chem. Inf. Comput. Sci., 1998. 38: p. 200-209.

21. Wessel, M.D., et al., Prediction of Human Intestinal Absorption of Drug Compounds from Molecular Structure. Molecular Modeling and Prediction of Bioavailability, 2000: p. 249-255.

22. Randic, M., Orthogonal Molecular Descriptors. New J. Chem, 1991. 15: p. 517-525.

23. Lucic, B., et al., The Structure-Property Models Can Be Improved Using the Orthogonalized Descriptors. J. Chem. Inf Comput. Sci., 1995. 35: p. 532-538.

24. NeuralWare, Predict 3.10. Feb 2003: Carnegie, PA15106-2700.

25. Sengers, J.V. Transport Properties of Fluids Near Critical Points. in Critical Phenomena. 1970. Villa Monestro: Academic Pres Inc. (London) Ltd.

26. Jagannathan, K. and A. Yethiraj, Moleucular dynamics simulations of a fluid near its critical point. Physical Review Letters, 2004. 93(1): p. 015701-1 to 015701-4.

27. Ohta, T., Multiplicative Renormalization of the Anomalous Shear Viscosity in Classical Liquids. J. Phys. C: Solid State Physics, 1977. 10: p. 791-793.

28. Bhattacharjee, K.J. and A.R. Ferrell, Critical Viscosity Exponent of a Classical Fluid. Physical Review A, 1983. 28(4): p. 2363-2369.

29. Berg, R.F. and M.R. Moldover, Critical Exponent of the Viscosity of Carbon dioxide and Xenon. J. Chem. Phys, 1990. 93(3): p. 1926-1938.

30. Stanley, E.H., Introduction to Phase Transitions and Critical Phenomena. The International Series of Monographs on Physics, ed. W. Marshall and D.H. Wilkinson. 1971, Oxford and New York: Oxford University Press.

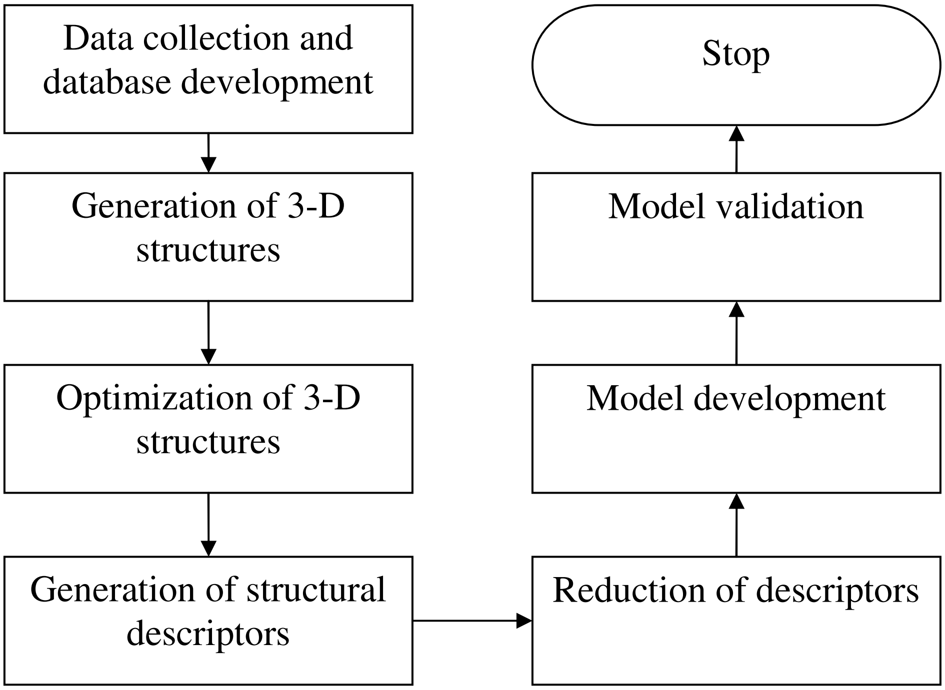

Figure 3.1. Overview of QSPR methodology [10]

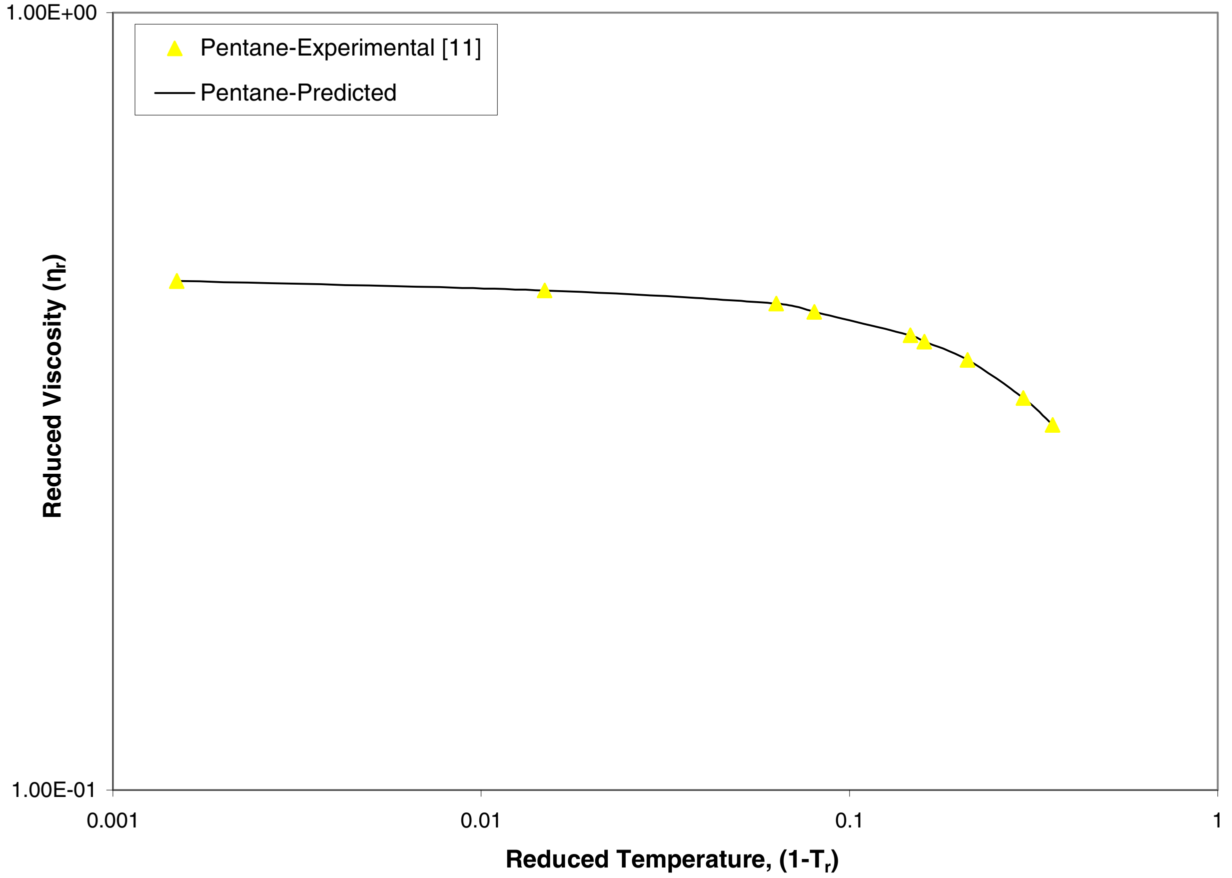

Figure 3.2. Variation of reduced vapor viscosity with temperature

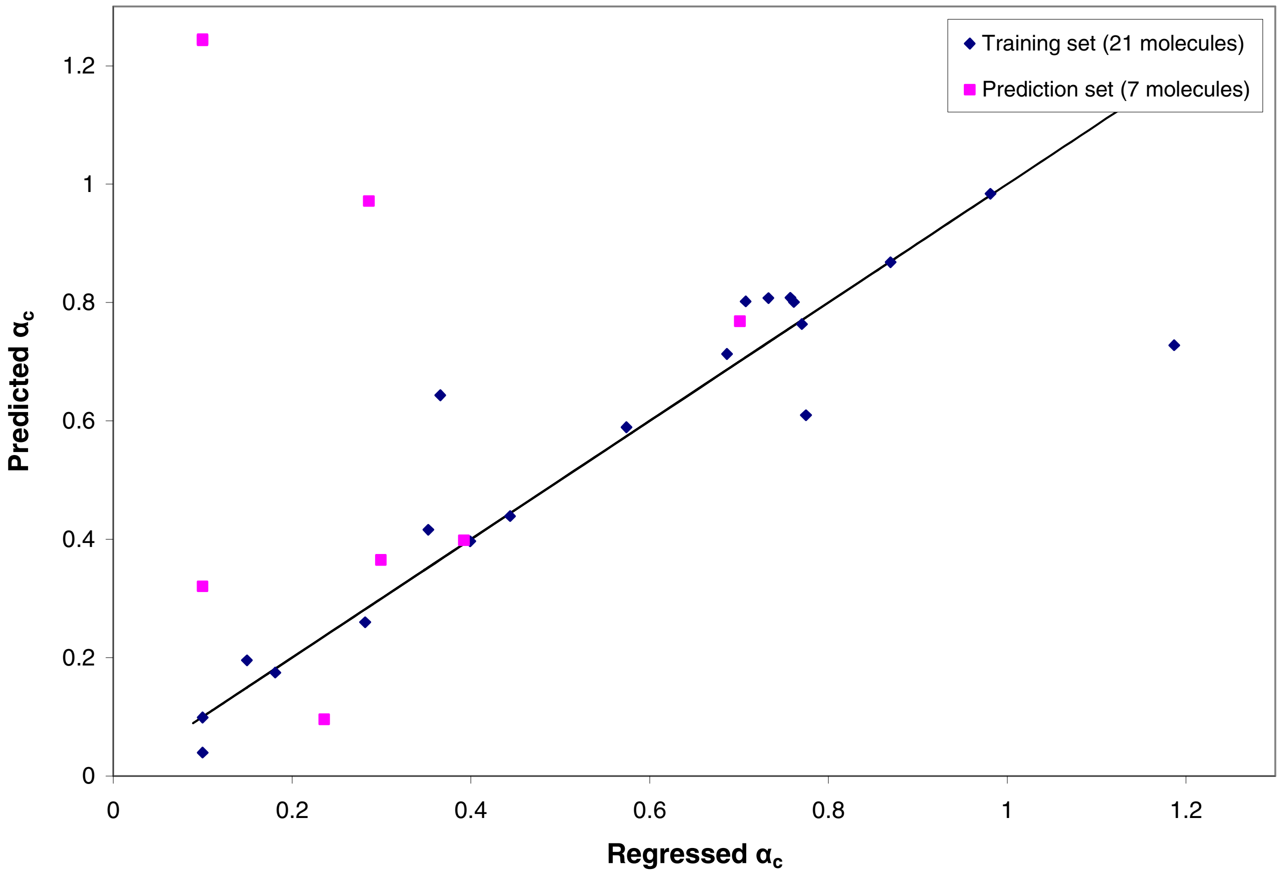

Figure 3.3. Comparison of regressed α_c and calculated α_c of the SVRC-QSPR model for vapor viscosity

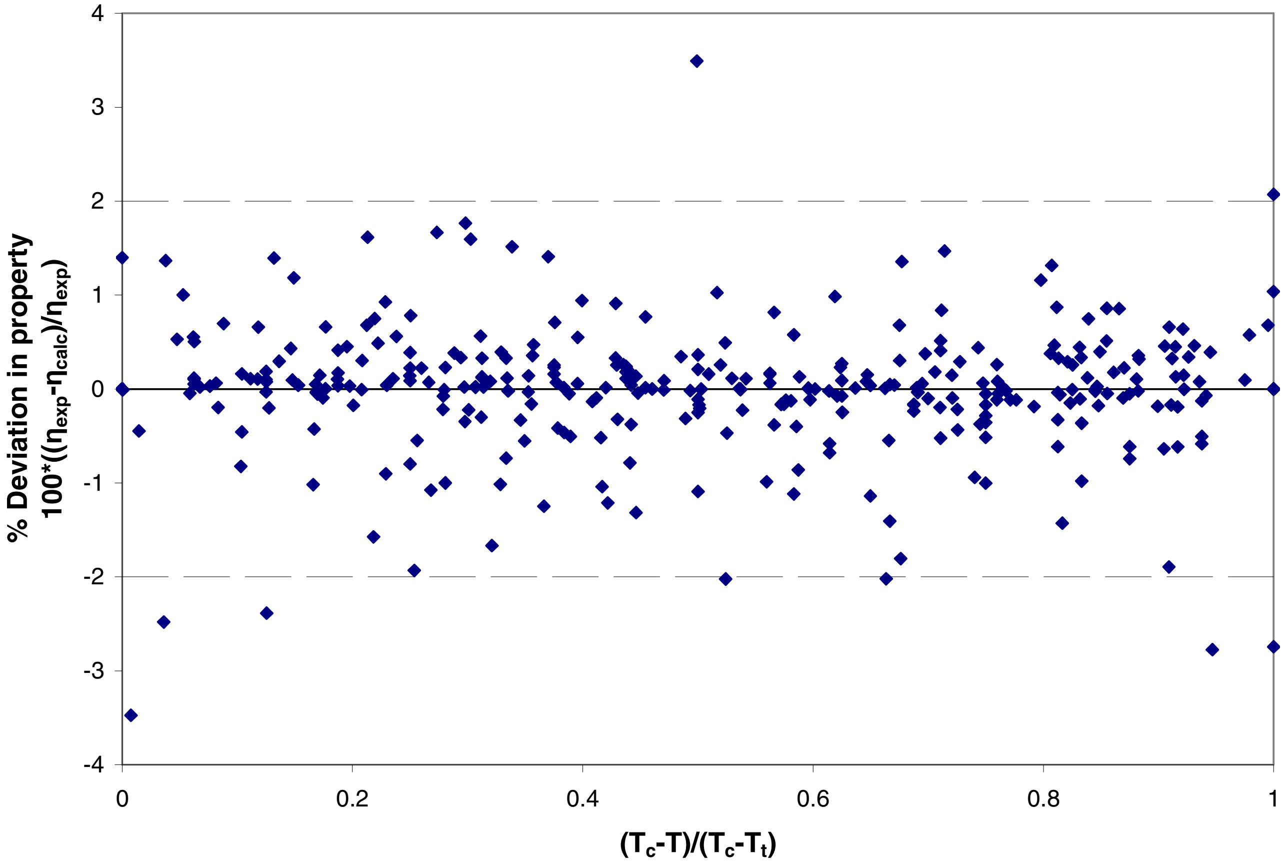

Figure 3.4. Deviations in regressed vapor viscosities using the SVRC model

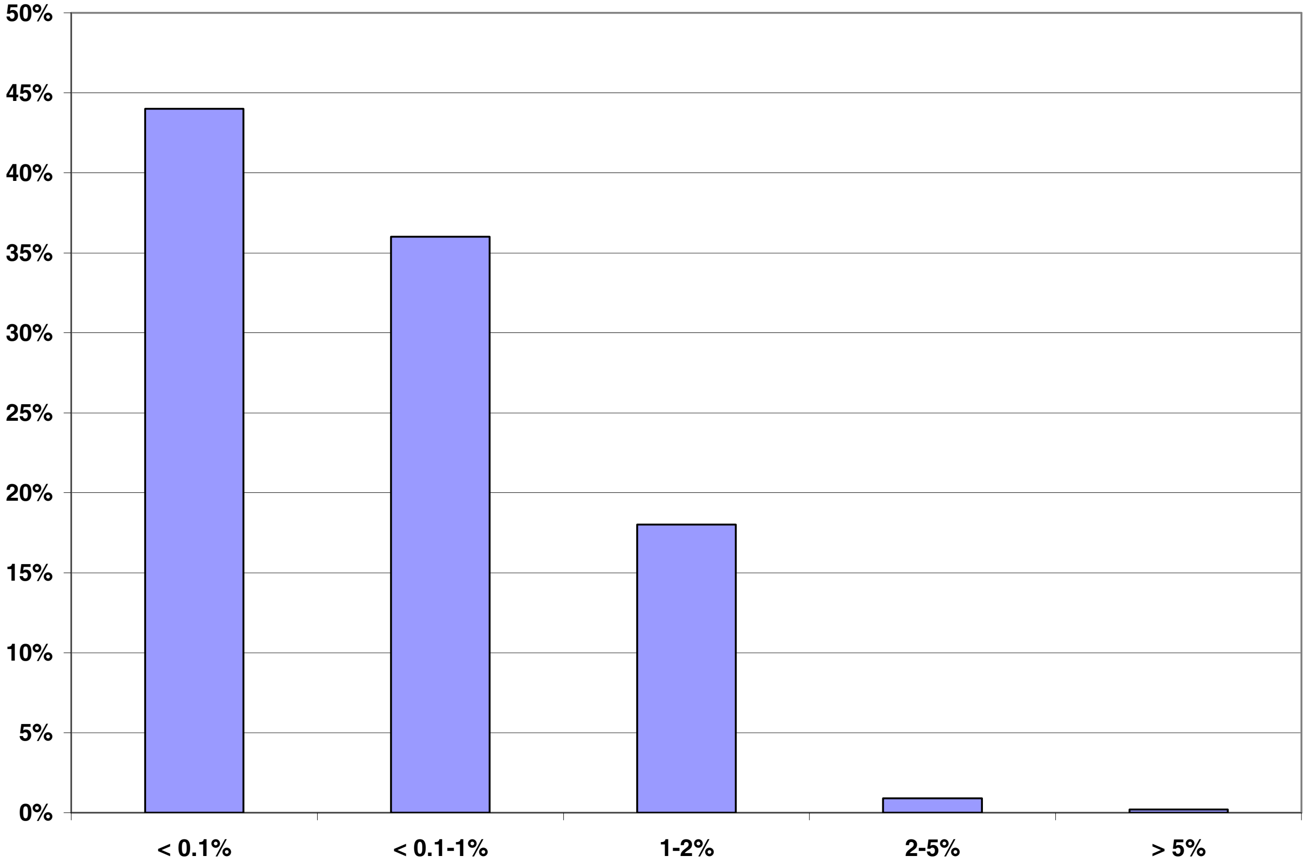

Figure 3.5. Distribution of errors (deviations) in predicted vapor viscosities using the generalized SVRC-QSPR model

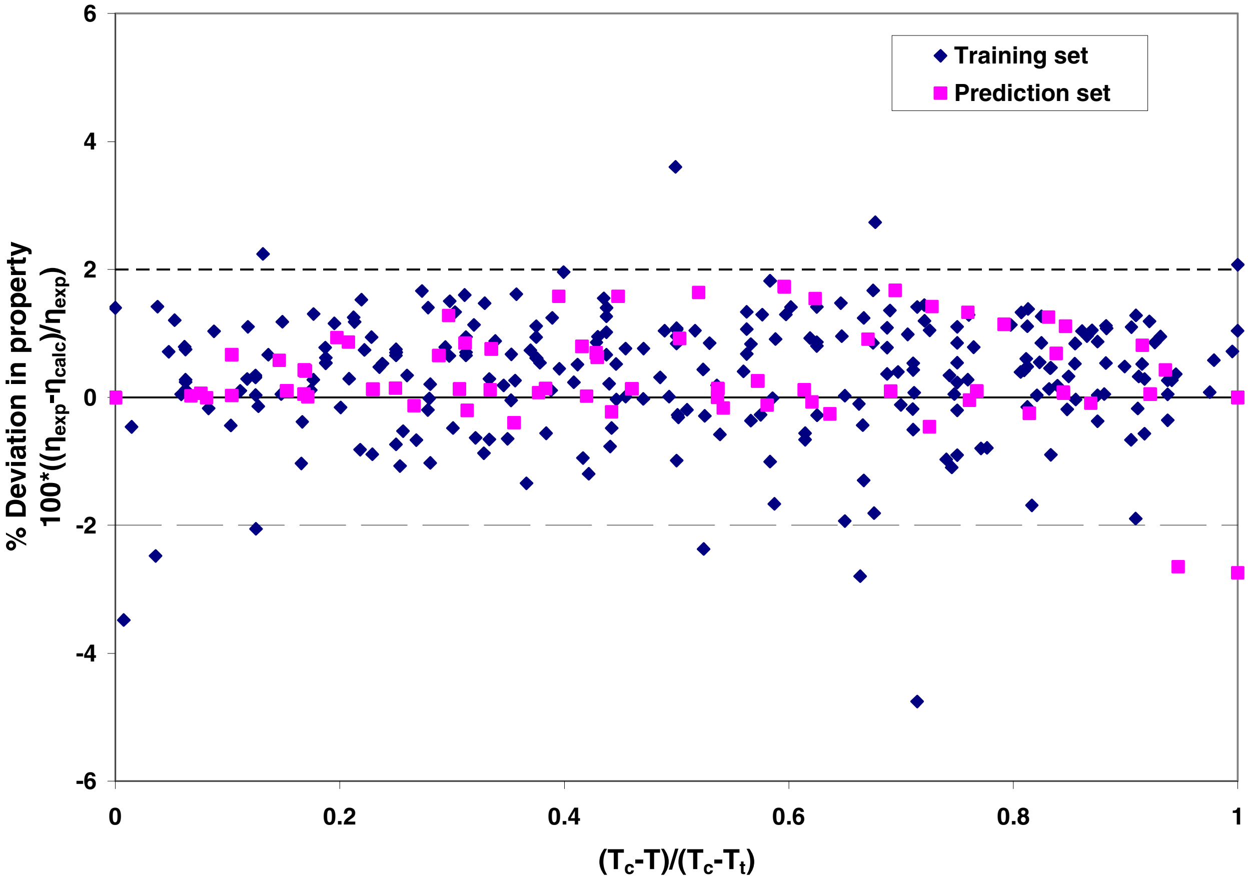

Figure 3.6. Deviations in predicted vapor viscosities using the generalized SVRC-QSPR model

Table 3.1. Predicted critical exponents characterizing the asymptotic temperature dependence for shear viscosity (η)

Investigator	η (varies as)	y	Basis	Year	Remarks	Reference
Fixman, Deutch, Mountain	ε^{-y}	0.5	Mean Field Theory	1962-67		[24]
Zwanzig	finite		Mean Field Theory	1967-68		[24]
Kadanoff and Swift	ε^{y}	$(\nu-\gamma+\alpha)/2$	Scaling Theory	1968-69	The value of the scaling exponent is 0.245	[24]
Kawasaki	ε^{-y}	0.5	Mean Field Theory	1969		[24]
De Sobrino	$\ln \varepsilon$		Mean Field Theory	1969		[24]
Kawasaki	$\ln \varepsilon$ or finite		Scaling Theory	1970		[24]
Ferrell	$\ln \varepsilon$ or finite		Scaling Theory	1970		[24]
Halperin and Hohenberg	ε^{-y}	0.043	Renormalization Group Theory		Since, $\xi \sim \varepsilon^{-\nu}$, where, $\nu = 0.63$	[25]
Ohta	ε^{-y}	0.031	Experimental	1977	Values calculated for the following fluids: Xenon and Ethane	[26]
Bhattacharjee and Ferrell	ε^{-y}	0.051	Mode-Coupling Theory	1983		[27]
Bhattacharjee and Ferrell	ε^{-y}	0.042	Mode-Coupling Theory	1986	Since, $\xi \sim \varepsilon^{-\nu}$, Where, $\nu = 0.63$	[27]

Table 3.1. Predicted critical exponents characterizing the asymptotic temperature dependence for shear viscosity (η) (contd.)

Investigator	η (varies as)	y	Basis	Year	Remarks	Reference
Berg and Moldover	ε^{-y*}	0.041	Experimental	1990	Values calculated for carbon dioxide and xenon	[28]
Berg, Moldover, and Zimmerli	ε^{-y}	0.043	Experimental	1999	Values calculated for xenon	[25]
Jagannathan and Yethiraj	ε^{-y}	0.043	Molecular Dynamics Simulations	2004	Since, $\xi \sim \varepsilon^{-\nu}$, where, $\nu = 0.63$	[25]

*ε is the symbol used for reduced temperature measured from the critical temperature T_c and is given by ε $|T-T_c|$ / Tc and ν, γ, and α are critical exponents of d=3 Ising model (fluid) with values of 0.638, 5/4, and 1/8 respectively [30].

Table 3.2. Summary of results obtained using regressed and predicted SVRC parameters

Compound Name	Case 1: %AAD of SVRC Model Regressions	Case 2: %AAD of Generalized SVRC-QSPR Model	Data points	Reduced Temperature Range (T_r)
PENTANE	0.3	0.4	9	0.64-1.00
HEPTANE, 2-METHYL-	0.4	1.0	7	0.64-0.98
HEPTANE, 3-METHYL-	0.1	0.1	6	0.63-0.97
HEPTANE, 4-METHYL-	0.8	0.8	6	0.64-0.94
NONANE	1.2	1.2	16	0.46-0.96
TRIDECANE	0.3	0.4	17	0.41-1.00
TETRADECANE	0.3	0.9	22	0.39-0.97
PENTADECANE	0.2	0.6	17	0.42-0.99
HEXADECANE	0.2	0.5	20	0.38-0.97
CYCLOPROPANE	0.7	0.7	21	0.74-1.00
CYCLOPENTANE	0.8	0.9	13	0.58-0.89
CYCLOHEXANE	0.4	0.4	13	0.58-1.00
ETHENE	0.05	0.1	8	0.68-0.97
1-PROPENE	0.3	0.4	21	0.53-0.97
BENZENE	0.5	1.1	49	0.51-0.98
BENZENE, METHYL-	1.0	1.1	15	0.56-0.89
SULFUR DIOXIDE	0.6	0.6	12	0.58-0.98
2-PROPANOL	0.2	0.2	9	0.77-0.97
ETHANE, CHLORO-	0.9	0.9	11	0.46-0.92
METHANE, CHLOROTRIFLUORO	0.7	0.7	6	0.81-0.99
METHANE, BROMO-	0.3	0.8	11	0.59-0.84
CARBON DISULFIDE	0.7	0.8	11	0.50-0.98
WATER-d2	0.2	0.8	11	0.43-0.58
R152A	0.02	0.1	35	0.63-0.97
R134A	0.1	1.1	14	0.65-0.92

Table 3.2. Summary of results obtained using regressed and predicted SVRC parameters (contd.)

Compound Name	Case 1: %AAD of SVRC Model Regressions	Case 2: %AAD of Generalized SVRC-QSPR Model	Data points	Reduced Temperature Range (T_r)
R32	0.1	0.1	13	0.64-0.98
R125	0.1	0.2	13	0.66-0.98
R124	0.02	0.4	14	0.68-0.83
Overall %AAD	**0.4**	**0.6**		

Table 3.3. Descriptors obtained from non-linear modeling of SVRC vapor viscosity model parameter α_c

Descriptors
Number of single bonds
Number of rings
Molecular volume/XYZ Box
Max partial charge for a H atom [Zefirov's PC]
WNSA-2 Weighted PNSA (PNSA2*TMSA/1000) [Zefirov's PC]

Table 3.4. Results of secondary validation for the generalized SVRC-QSPR model using an external dataset

Chemical classes represented in the training set	%AAD	Datasets
METHYLALKANES	3.4	17
N-ALKANES	4.6	29
CYCLOALKANES	1.2	6
1-ALKENES	1.9	20
N-ALKYLBENZENES	2.2	15
INORGANIC GASES	2.9	8
OTHER ALIPHATIC ALCOHOLS	1.2	30

Table 3.5. Results of secondary validation for the generalized SVRC-QSPR model using an external dataset

Chemical classes not represented in the training set	%AAD	Datasets
TERPENES	1.3	8
2.9	2.9	20
ACETATES	4.1	12
ALDEHYDES	1.6	28
ALKYLCYCLOHEXANES	1.1	17
ALKYLCYCLOPENTANES	0.9	11
ALKYNES	2.6	17
ANHYDRIDES	2.3	8
AROMATIC ALCOHOLS	1.3	16
AROMATIC CARBOXYLIC ACIDS	2.8	4
AROMATIC ESTERS	6.5	3
CYCLOALIPHATIC ALCOHOLS	0.4	10
CYCLOALKANES	1.2	6
CYCLOALKENES	1.3	15
DIALKENES	1.5	26
DICARBOXYLIC ACIDS	0.9	4
DIMETHYLALKANES	1.5	16
DIPHENYL/POLYAROMATICS	2.7	19
ELEMENTS	2.7	4
ETHYL & HIGHER ALKENES	2.0	12
FORMATES	0.6	10
INORGANIC GASES	2.9	8
KETONES	1.5	33
POLYFUNCTIONAL ACIDS	3.4	17
METHYLALKENES	1.6	16
MULTIRING CYCLOALKANES	0.5	3
N-ALCOHOLS	1.2	20
N-ALIPHATIC ACIDS	1.8	15
POLYFUNCTIONAL C, H, O, N	3.5	2
POLYOLS	2.7	35
NAPHTHALENES	1.5	15
OTHER ALIPHATIC ACIDS	4.6	16
PROPIONATES AND BUTYRATES	3.8	9
OTHER ALKANES	3.6	25
OTHER ALKYLBENZENES	1.4	46
OTHER CONDENSED RINGS	0.5	10
OTHER ETHERS/DIETHERS	0.3	2
OTHER HYDROCARBON RINGS	0.5	16
OTHER MONOAROMATICS	1.8	19
OTHER POLYFUNCTIONAL C, H, O	0.9	3
OTHER SATURATED ALIPHATIC ESTERS	3.6	7

CHAPTER 4

SVRC-QSPR MODEL FOR SURFACE TENSIONS

Introduction

Surface Tension (ST) is of importance for many processes and phenomena, such as gas injection displacement, flow through porous media, mass and heat transfer. Liquid/vapor surface tensions need to be accurately predicted because they control processes in which the liquid phase is finely dispersed. For instance, the parameters characterizing the transport of vapor (gas) or liquid (oil) in a porous medium (such as capillary pressure, relative permeabilities and the residual liquid saturation), are strongly dependent on the ST. ST values are, thus, necessary to simulate compositional and gas injection processes in petroleum recovery. At low values, it is the dominant fluid property which determines relative permeabilities and residual liquid saturations in gas condensate systems. Favorable recovery conditions of high relative permeabilities and low residual condensate saturations have been found at STs less than 0.1 mN/m. The low ST region occurs near the critical point. There are very few experimental results in this region to test the effectiveness of correlations to predict STs.

The correlations available in the literature for predicting ST currently have a limited range of applicability or poor suitability for generalization. Further, most of the literature models exhibit large errors near the critical point of the fluid and rely on experimentally measured physical properties as input for their predictions. Although experimental data are available in the literature for several compounds that have been already investigated, there arises a need for a generalized model capable of providing *a priori* predictions for compounds yet to be synthesized.

Previously, researchers at Oklahoma State University (OSU) have developed a unified framework for correlating saturation properties, which includes vapor pressure, liquid and vapor densities [1, 2]. This scaled-variable-reduced-coordinates (SVRC) model is based on the corresponding states theory (CST) and scaling-law behavior and in general is capable of representing saturation properties within their experimental uncertainties. In this work, we attempt to extend the SVRC model to correlate ST and generalize the model parameters using structure-property modeling. A database of 2829 data points involving 198 fluids was used to develop this model. When the model was applied to an external dataset containing 10,951 data points involving 685 fluids, the ST data were predicted, on average, within 5% of the reported values. The approach involves the use of QSPR methodology to generalize the model parameters of the developed SVRC model. Specifically, we use SVRC to develop the behavior model, and QSPR to generalize the SVRC model parameters. This approach, in the past, has proven to be more effective than the typical efforts to develop generalized models directly using QSPR techniques [see, e.g., 3].

Surface Tension Prediction Models

Several models are available in the literature for prediction of ST. While most of these models are empirical in nature, there are some which have a sound theoretical basis. Among the earliest works, MacLeod (1923) suggested that the ST can be expressed in terms of the liquid and vapor densities by the following equation [4]:

$$\sigma^{1/4} = P\left(\rho^{L} - \rho^{V}\right) \tag{1}$$

where P is a temperature independent parameter and ρ^L and ρ^V are the liquid and vapor densities, respectively. Sugden (1932) named the parameter P as the parachor and proposed that it can be estimated from structure. The parachor equation has been the most widely used equation in the industry.

Over the years, various methods for estimating the parachors for pure fluids have been proposed in the literature. Quale used experimental values of ST and density to estimate the parachors using an additive scheme to correlate them with molecular structure. The values of P calculated using this scheme are listed elsewhere [4]. Fanchl in 1990 proposed a correlation for estimating parachors of high molecular weight compounds [5]. Ali in 1995 made a comparison of seven existing correlations available for parachor estimation and proposed his own to estimate the parachors of C7+ compounds and other pseudo components [6]. Schechter in 1995 back-calculated the parachors of 139 compounds using ST and density data obtained from experiments conducted by previous investigators [7]. Broseta in 1995 used critical scaling theory to relate the parachor of a pure compound to its critical temperature, critical pressure and acentric factor [8]. Zuo and co-workers developed a generalized corresponding states model based on two reference fluids and a parachor-correlation for prediction of interfacial tensions of non-polar and weakly-polar pure fluids and mixtures [9]. Cumber developed an improved parachor correlation for ST prediction of hydrocarbons based on fluid composition [10].

Various modifications to the parachor equation have been proposed by researchers extending it to multi-component mixtures. Gasem and co-workers [11] made a comparative study of three commonly used correlations that are based on the parachor equation for prediction of ST of multi-component mixtures and suggested the use of 3.6 as the value of scaling exponent as opposed to the value of 4.0 used in Equation 1. Although widely used, the parachor equation requires the values of liquid and vapor densities for ST prediction. An equation of state would normally be used to compute these values in case experimental values are not available. However, equations of state currently available in the literature do not give accurate and reliable predictions of liquid and vapor densities. The errors in computation of these values would translate into larger errors in the values of predicted ST. Dandekar [12] studied the qualitative and quantitative effects of such inaccuracies in ST predictions. From his study, he concluded that an error of 10% in liquid or vapor density can result in an error up to 200% in the estimated ST. This raises doubts about the reliability of the parachor equation. A review of various other empirical correlations used to predict ST is detailed elsewhere [4].

Other theoretical methods to correlate and predict ST are based on the following theories: corresponding states theory, Gibbs method, perturbation theory, integral equation theory, density gradient theory and the density functional theory (DFT) [13]. Lu and co-workers [13] used the Barker–Henderson (BH) perturbation theory and statistical associating fluid theory (SAFT) to develop a thermodynamic method based on the DFT to predict the ST of polar and associating fluids. The STs for four pure non-associating polar fluids and 11 associating fluids over a wide temperature range were predicted with an average deviation of 2.9%. Do and coworkers [14] used the molecular structure theory to describe ST. They modeled the fluid as a set of mono-layers and accounted for interaction among molecules in a layer and the interaction between layers [14]. Recently, Esposito and co-workers proposed a correlation that accounted for the effect of interfacial curvature on ST [15].

Most of the above-mentioned models available in the literature rely on experimentally measured physical properties as input for their predictions. Although experimental data are available in the literature for several compounds that have been already investigated, there arises a need for a generalized model capable of providing *a priori* predictions for compounds that are yet to be synthesized. This requires the establishment of a relationship between the ST of the liquid and its chemical structure. The use of quantitative structure property relationship (QSPR) is one such approach where models are obtained on the basis of the correlation between the experimental values of the property and descriptors reflecting the molecular structure of the respective compounds.

Kavun and co-workers in 1995 evaluated over 450 molecular descriptors in developing a QSPR model for ST and proposed an eight-descriptor model that fitted ST data of 72 organic chemicals with an R^2 value of 0.955:

$$ST = 37.4 - 690.6\frac{q_{\max}}{N} - 264.5\frac{q_{\min}}{N} + 401.95\frac{\Sigma q(Hal)}{N} - 2.05S_S - 1.08\frac{S_{uns}}{N} + 1.04\ln(1+S_P) + 67.8{}^{i}\chi^{v}$$

where, *q*max and *q*min are maximal and minimal charges on the atoms; Σ*q*(Hal) is the net charge on halogen atoms; S_s and S_{uns} are the surface area of saturated and unsaturated apolar surface of the molecule; S_p is the area of the polar van der Waals surface; N is the number of atoms, and ${}^{i}\chi^{\hat{\imath}}$ is the valence index of connectivity. However, when the model was applied to an external testing set of 22 chemicals, the ST data were predicted within 30% of the measured values [16]. Egemen and coworkers [16] proposed a group contribution method employing a multiple step-wise linear regression procedure to predict ST of liquid organic solvents:

$$ST = 16.36 + \sum_{i=1}^{i=m} \left(n_i * contribution_i \right)$$

where, m represents the number of various types of atoms/bonds and n represents the count of each type of atom/bond in the molecule. The proposed model was developed using a training set of 349 chemicals which could fit the experimental ST values with a R^2 value of 0.75. The model was then used to predict the ST of an external testing set consisting of 44 chemicals. The model could predict the ST values of the testing set with a R^2 value of 0.89. Although the model seems promising, the predictions were obtained over a narrow temperature range of 20-30^0 C and the model could predict ST values within ~10% of the measured values.

Kaufmann and coworkers [17] proposed an eight descriptor model for predicting the ST of 213 common organic solvents. Their linear model developed using multi-linear regression (MLR) technique had training set R^2 value of 0.914 and a prediction set R^2 value of 0.915. Their non-linear model developed using 8-6-1 neural network architecture had a training set R^2 of 0.965 and a prediction set R^2 value of 0.976. The average percent error of the predictions using this model was 5.3% for the training set, 6.1% for the cross-validation set, and 6.4% for the prediction set. Knotts and co-workers [18] proposed to improve the Macleod-Sugden-Quayle (MSQ) method for predicting ST. They coupled experimental ST data from DIPPR database and TSAR (a commercial QSPR software package) to predict parachors used in the MSQ method. The values of liquid density and vapor density used in estimating the parachors were obtained from the DIPPR correlation and the Soave equation, respectively. The improved correlation could fit the experimental ST values for 649 compounds with an AAD of 3.2%.

A thorough review of the literature suggests that most of the predictive methods found in the literature are restricted to a narrow range of compounds and temperatures. Few of these models are generalized and applicable over the entire saturation range. Furthermore, the accuracy and reliability of these are difficult to state because the testing methods adopted by the different authors lack a common database and the range and applicability of the testing have not been stated in the literature. In addition, most of these models present large deviations in the near critical region. Hence there arises a need for a generalized model utilizing minimum number of parameters capable of predicting the ST of pure fluids over the entire saturation range (triple to critical point).

Scaled-Variable-Reduced-Coordinate Framework

In previous studies [1, 2], the SVRC framework was used to correlate saturation properties of a wide variety of organic molecules over the entire saturation range. The SVRC model utilizes corresponding states theory (CST) and scaling-law behavior.

The general SVRC framework for correlation of thermo-physical properties is given as [1, 2]:

$$\left(Y_\infty^\alpha - Y^\alpha\right)\Big/\left(Y_\infty^\alpha - Y_0^\alpha\right) = \Theta(\varepsilon) \qquad (1)$$

or

$$Y^{\alpha} = Y_0^{\alpha}\Theta(\varepsilon) + \left[1 - \Theta(\varepsilon)\right]Y_{\infty}^{\alpha} \tag{2}$$

where,

$$\varepsilon = \left(X_{\infty} - X\right)/\left(X_{\infty} - X_0\right) \tag{3}$$

$\Theta(\varepsilon)$ is the correlating function, X is the correlating variable, Y is the saturation property at given X, Y_{∞} is the asymptotic value of saturation property at X_{∞}, Y_0 is the initial value of saturation property at X_0 and α is the scaling exponent.

To correlate saturation properties, Equation (1) is recast for representing the various properties between the triple and the critical points as:

$$Y = \left\{Y_c^{\alpha} - \left(Y_c^{\alpha} - Y_t^{\alpha}\right)\Theta\right\}^{(1/\alpha)} \tag{4}$$

Since, the ST becomes zero at the critical point, the ST correlation is written as:

$$\sigma = \sigma_t \Theta^{1/\alpha} \tag{5}$$

where, σ_t is the ST at the triple point. In this work, due to restricted availability of data, the ST at the lowest available temperature was taken to be σ_t for modeling purposes.

The functions $\Theta(\varepsilon)$ and α are defined as:

$$\Theta(\varepsilon) = \frac{\left(1 - A^{\varepsilon^B}\right)}{\left(1 - A\right)} \tag{6}$$

$$\alpha = \alpha_c \tag{7}$$

where

$$\varepsilon = \frac{T_c - T}{T_c - T_t} \tag{8}$$

A, B and C are correlation constants; α_c is the limiting value of α at the critical temperature. The SVRC model accounts for the effects of temperature and chemical structure through the correlating function (Θ) and the scaling function (α).

QSPR Methodology

Computational techniques have gained popularity recently owing to the advances in technology. They are increasingly used to address complex engineering and design problems in chemical processing. The QSPR approach is among the computational methods gaining wide use. It is based on the assumption that there exists a relationship between the structure of a substance and its physical and chemical properties. QSPR uses quantum mechanics to define the structure of the molecule in terms of a series of molecular descriptors and then correlates the property in terms of these descriptors. The following steps are part of any QSPR model development effort [19] (a) generation of 3-D structures, (b) optimization of 3-D structures, (c) calculation of descriptors, (d) reduction of descriptors, and (e) development of a QSPR model. Figure 4.1 describes the procedure followed in the QSPR modeling effort undertaken. The procedure used to develop QSPR generalization for the SVRC model parameter (α_c) is outlined in the following paragraphs.

Database Development

A property database of pure fluids including a wide range of compounds belonging to diverse chemical classes was used in the SVRC surface tension model development. The data used in this study were gathered mainly from the DIPPR database

[20] and a compilation by Jasper [21]. A database containing 2901 data points involving 200 fluids was used in the model development. This database was screened to include only fluids for which quality experimental data (with reported errors of less than 5%) were available. Also, only datasets with more than eight data points were included in the model development procedure. To the extent possible, for each compound, we sought data that covered a wide temperature range in the saturation region. Data points with %AAD (absolute average deviation) greater than thrice the overall regression %AAD (~ 5%) of a compound were eliminated from the database in an effort to remove data with relatively large uncertainties. Based on this procedure, a total of 72 data points were eliminated which constituted about 2% of the total. The reduced database finally contained 2829 data points involving 198 fluids. A list of the compounds used and the reduced temperature ranges for each molecule can be found in Table C.1 of Appendix C.

Structure Generation

The first step in any QSPR modeling effort is the generation of chemical structures. Various kinds of chemical representation have been proposed in the literature. The most common way of representing a chemical is a two-dimensional (2-D) sketch [19]. But, the drawback of using a 2-D representation is that it does not provide a complete description of the molecule and cannot be conveniently used for database storage and searching [19]. To have an efficient QSPR model, the representation of a molecule should provide all the necessary structural information. This requires information about the atoms present, along with three-dimensional (3-D) coordinates that provide a full spatial depiction of the molecule. A commercial package, ChemDraw [22] was used to generate the 3-D structures of the molecules.

Structure Optimization

More than one set of 3-D coordinates can be generated for any given molecule. Most molecules contain single bonds that join two groups of atoms. Such bonds can usually rotate with a low-to-moderate energy barrier that changes the orientation of other groups in the structure and thereby the value of the descriptors [19]. In nature, all these representations occur in differing probability and the objective of structure optimization is to obtain a 3-D structure which is most prominent and has the minimal potential energy surface. In this work, the 3-D structures generated were first optimized using the MOPAC and MM2 routines available in the ChemDraw package and later using another commercial optimization software called AMPAC [23]. The use of two optimization routines practically eliminated any un-optimized structures. Intricate details of 3-D structure generation and optimization are beyond the scope of this work. A detailed explanation can be found elsewhere [19, 23].

Descriptor Generation

Once an accurate 3-D structure of a chemical has been obtained, the next step involves calculation of the molecular descriptors. The molecular descriptors calculated by any commercial package are usually divided into (1) constitutional, (2) topological, (3) geometrical, (4) electrostatic, (5) quantum-chemical and (6) thermodynamic. Details about these classes of descriptors can be found elsewhere [19]. In this work, commercial software called CODESSA [24] was used to generate the descriptors. Around 400 descriptors were generated for each molecule. The actual number of descriptors calculated for each molecule varied based on the structural complexity of the molecule.

Descriptor Reduction

All the 400 descriptors generated for each molecule are not significant in modeling ST. The use of all available descriptors in the model development effort causes dimensionality problems. Further, the use of irrelevant or redundant descriptors diminishes the performance of a QSPR model, especially when non-linear algorithms are used in model development. Descriptor reduction (DR) is the process of automating the discovery of potentially useful correlations from large sets of descriptor data [19]. The DR process involves the identification of the most relevant set of descriptors for model development and is the most important step in all QSPR model development efforts. Several different methods for DR are available in the literature. The most widely used techniques are the principal-component analysis (PCA), partial least-squares (PLS), genetic algorithms (GA), and neural networks (NNs) [19].

Most QSPR models developed have been based on multiple linear regression correlations requiring *a priori* assumption of the form of the mathematical correlation model. Such models do not consider the non-linearity that may exist among the input parameters and the output properties. The above deficiencies have been addressed in the past using Artificial Neural Networks (ANN). Neural networks are powerful tools for correlating, predicting and classifying large complex data sets. It can successfully deal with non-linearity, handle noisy or irregular data, correlate hundreds of variables or parameters, and provide generalized solutions [25]. However, commonly-used neural network architectures, such as back propagation networks, demand extensive training (using a significant amount of data) to develop a stable QSPR model [26]. This places further demands on modeling efforts since reliable experimental data are not easily available. Another Artificial Intelligence (AI) tool that has been used in QSPR model development are the Genetic Algorithms (GA) [27, 28]. Genetic search methods are based on Darwinian models of natural selection and evolution. The general idea behind GA is the evolutionary creation of a new population of entities from an earlier generation through crossover and mutation processes and by passing on the fittest offspring to the next generation [29]. This approach is ultimately expected to lead to generations that become fitter through evolution thereby achieving the desired objective. More details on GA can be found elsewhere [29].

Hybrid approaches using genetic algorithms and neural networks have also been recently proposed, and have shown good promise in developing accurate and robust QSPR models [30, 31]. In this work, such a hybrid approach employing Genetic Algorithms and Neural Networks was used to develop a generalized non-linear model for STs.

QSPR Model Development

This work aimed at (a) demonstrating the ability of the SVRC model to precisely represent ST using one regressed parameter, (b) examining the efficacy of using QSPR algorithms to obtain estimates for the SVRC parameter based on chemical structure information using non-linear algorithms. Two case studies were conducted in sequence to achieve these objectives:

Case 1. Determination of the SVRC parameter (α_c) by regressing experimental data

Case 2. Generalization of the SVRC parameter using non-linear structure-based models

The ST model development was initiated with the regression of the SVRC parameter for each molecule (Case 1). As can be seen from Equations 5-7, the SVRC model for ST has four parameters A, B, C, and α (α_c.in this case) Amongst these, A, and C are treated as universal constants applicable to all fluids. Based on regression, the values of these constants are fixed to be the following: A=1.0004; C=1.33. B is the universal scaling exponent, which characterizes the divergence of ST near the critical point. Based on a thorough literature review, a widely accepted value for this exponent, 1.26, was chosen as the value for B. As shown in Figure 4.2, this combination of constants provided good representation of the data. The other parameter, α_c was treated as substance specific. A rigorous generalization strategy based on chemical structure information alone was adopted.

Structure-based model development was initiated with structure generation, optimization, and descriptor generation. Studies have shown that structural descriptors are often highly correlated leading to numerical instabilities commonly referred to as multi-collinearity. In such instances, it becomes increasingly difficult to disentangle the unique effects of each predictor (descriptor) on the response variable. Multi-collinearity results in highly unstable estimated regression coefficients, the values of which are extremely sensitive to addition/removal of variables or small changes in data points leading to erroneous results and interpretations [32]. To tackle this problem, the use of orthogonal molecular descriptors is suggested by studies in the literature. The procedure of orthogonalization focuses on the residuals of intercorrelation between descriptors thereby ensuring that distinct structural characteristics of various descriptors are extracted and used as novel descriptors, which are free from mutual relatedness [32]. More information on the procedure of orthogonalization and its use can be found elsewhere [32, 33]. In this work, the descriptors generated by CODESSA were orthogonalized to obtain a subset of descriptors from which all redundant information has been removed. Non-linear DR techniques were then applied to this reduced subset of descriptors.

The non-linear modeling was performed using commercial software [34]. The reduced subset of descriptors obtained from the orthogonalization step is exported to the software which has a Microsoft Excel™ interface. The software employs GA to identify the best set of input variables for the model. A GA operates on a population of individuals. The population changes from one generation to the next, usually by combining characteristics of two "parent" individuals to create a "child" individual. Every individual is assigned fitness and the concept of "survival of the fittest" is implemented by selecting the fit parents more frequently than less fit parents to create the next generation [34].

In this case, an "individual" is actually a set of descriptors. The fitness of a descriptor is derived from the performance of a model that uses the descriptor's variable set as inputs. The algorithm begins with descriptors that consist of small sets of variables. Descriptors that produce good models are kept in the population and used to generate descriptors that consist of larger sets of variables if necessary. In general, however, smaller variable sets (that is, fewer model inputs) are preferred to larger variable sets. The fitness of a descriptor is evaluated using Neural Networks. The software constructs the actual neural network incrementally, using a technique known as cascade correlation. Hidden units are periodically added, usually one or two at a time. Each time a hidden unit or pair of hidden units is added, weights are trained from several different initialization values. Each initialization is referred to as a candidate. The best candidate is established in the network, and then all the weights to the output node(s) of the network are retrained.

There are several heuristics that provide guidance as to the permissible number of hidden neurons or choice of networks weights and criteria for termination of training. For example, when determining the network architecture, the rule of thumb is to keep the ratio of total observations (number of molecules) to adjustable parameters (network weights) above two to avoid any chance effects. However, these rules are just approximations and trial-and-error investigation remains a reliable method for choosing the best parameters [3]. After rigorous trial-and-error analysis, a 12-1-1 (12 descriptors-1 hidden neurons-1 output variable) architecture was adopted for the parameter α_c. To validate the neural network model, the data set containing 198 molecules were randomly split into training and prediction (test) sets. The prediction and training sets contained 30%, and 70% of the data, respectively. The SVRC parameter for ST was predicted using the final network obtained after training and cross validation. The predicted parameter was then applied in the SVRC model (Equation 5). The extent of training and the stability of the neural network model were validated based on the quality of the model predictions obtained (overall %AAD).

Results and Discussion

Table 4.1 presents the summary results for the case studies conducted. The entire data set containing 198 molecules was correlated using a one-parameter SVRC model. As indicated by the results for Case 1, the SVRC model represents the STs of the diverse organic subset over a wide temperature range in the saturation region, with AAD of 0.6% using one regressed parameter.

The SVRC parameter was then generalized using non-linear QSPR models (Case 2). A hybrid approach employing Genetic Algorithms and Neural Networks was used to identify the best non-linear model that provided accurate predictions. GA was used to identify the best subset of descriptors and NN was used to evaluate the fitness of the selected individuals (descriptors). A sigmoidal transfer function was used and several architectures were investigated by varying the number of hidden neurons. A 12-1-1 architecture for the parameter α_c was found to provide the best performance as measured from the overall %AAD of the property predictions from the model. The numbers of adjustable parameters in the network architecture for the model parameter was also found to obey the above mentioned heuristic (ratio of number of systems used for training to the number of adjustable parameters being greater than two). The descriptors generated from the non-linear model can be found in Table 4.2.

Analysis of our preliminary prediction results for Case 2 indicated that there were 13 molecules which had large prediction errors (>2% AAD), which include (a) hexane (2.5% AAD), (b) 1, 1, 3, 1-Terphenyl (3.4% AAD), (c) 3-pentanone (3.0% AAD), (d) methanol (3.1% AAD), (e) ethanol, 2-Butoxy (2.3% AAD), (f) ethane, 1,1'-Oxybis, 2-Chloro- (4.6% AAD), (g) 1-hexanamine (6.4% AAD), (h) hydrogen (7.4% AAD), (i) acetic anhydride (3.8% AAD), (j) methyl formate (3.6% AAD), (k) isobutane (4.1% AAD), (l) 1-pentanol, 3-methyl (4.3% AAD), (m) cyclopentene (4.1% AAD), (n) ethanol, 2-amino (4.1% AAD). These 15 fluids were isolated for further analysis. The source of prediction errors was surmised to be the choice of critical propertied used. Previous studies in the literature [3] have discussed the influence of errors on critical temperature on model stability and have suggested that critical temperatures could vary as much as 3%, depending on the apparatus and operating procedures. Therefore, when a 3% variation was allowed in the critical temperature, a reduction in errors was noticed. The overall AAD for the 198 fluids reduced to 1.2% from 1.4%.

Figure 4.3 shows a comparison between the regressed SVRC parameter and the SVRC parameter predicted from structure using the non-linear QSPR model. Figure 4.4 shows the percentage deviations in vapor viscosities obtained from data regressions using the SVRC model. The prediction results for the STs are depicted in Figures 4.5-4.6. Figure 4.5 shows the percentage distribution of errors in the predicted STs. On average, the SVRC model was capable of representing the STs with an AAD of 0.6% and the generalized SVRC-QSPR model was capable of predicting the STs with an AAD of 1.2%. For developing the non-linear model, the entire dataset was divided into training and prediction sets each containing 70% and 30 % of the data, respectively. Figure 4.6 represents the percentage deviations in STs for the training and the prediction sets with respect to the reduced temperature. From Figure 4.5, it is evident that the generalized SVRC-QSPR model predicts the STs of the majority of the data points with an AAD of 2%.

To further validate the predictive capability of the SVRC-QSPR model, an external data set from the DIPPR database that was not included in the model development was used. The external dataset comprised of 7048 data points involving 687 fluids. A list of the molecules used for the external validation is provided in Table C.2 of Appendix C. This dataset differed from the one that was used for model development in *that it primarily contained ST values that were obtained from other predictive models and smoothing functions* (as reported in the DIPPR database) and was not screened for quality based on reported errors. The limited experimental data contained in this database did not meet the screen criteria of the primary database used for model development. The external dataset contained 47 classes of compounds of which 28 had representation in the training set used in model development.

The data in the external dataset were culled to separate the classes of compounds that had representation in the training set from the ones that did not. The generalized SVRC-QSPR model was initially applied to fluids belonging to chemical classes which had representation in the training set (3743 data points involving 213 fluids (datasets)). The predictions obtained from the model were compared to the values reported in the external dataset. However, fluids belonging to some classes of compounds, mainly, 'N-Alkylbenzenes', 'Methylalkanes', and 'Methylalkenes', 'n-Alcohols', and 'Aromatic Esters' exhibited large prediction errors (>10% AAD). This might be attributed to the fact that there was not adequate representation for these classes of compounds in the training set. For example, in the case of 'Aromatic Esters', the training set had simple fluids like 'benzoic acid, methyl ester, benzoic acid, ethyl ester, and benzoic acid, phenylmethyl ester', while the external dataset contained structurally more complex aromatic esters (for example, '1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester, 1,2-benzenedicarboxylic acid, di-isooctyl ester' etc.). Table 3.5 shows the AADs obtained for the different classes of compounds in the external dataset that had representation in the training set. The generalized model was then applied to fluids belonging to chemical classes that did not have representation in the training set (3743 data points involving 429 fluids). The results for the same are presented in Table 3.6. In general, the generalized SVRC-QSPR model was capable of making *a priori* predictions for the compounds in the external database with an overall AAD of ~6%.

With few exceptions, in general, the classes of compounds that are represented in the training set have lower prediction errors than the ones that do not have representation. Although, the secondary validation process provides valuable insights regarding the predictive ability of the developed generalized SVRC-QSPR model, only a guarded judgment can be made based on this study since majority of the ST values reported in the external dataset mostly come from other predictive models and smoothing functions with relatively high reported errors.

The primary goal of this study was to develop a generalized ST model capable of providing accurate *a priori* predictions (a) over a wide temperature range in the saturation region, and (b) for a diverse set of molecules involving various functional groups. Our model provides good ST representations (AAD of 0.6% for 198 molecules) and predictions (1.2% AAD) in comparison to other recommended literature models which in general are capable of providing predictions within 5-10% [35]. The predictions obtained were compared to the models recommended in the literature [5]. The results obtained for selected polar and non-polar compounds are presented in Tabled C.3 and C.4 of Appendix C. A favorable comparison is indicated for the SVRC-QSPR model.

As evidenced by the results, the generalized SVRC-QSPR model is capable of correlating/predicting the STs of a diverse set of molecules with varying structural complexities. Also, our work attempts to model STs over a wide temperature as opposed to the currently available QSPR models which are restricted to single temperature (298 K) predictions [17, 18].

In this study, we hypothesized that an approach, which calls for the use of theory to develop the behavior model, and QSPR to generalize the parameters of such model, is more effective. The quality of the ST predictions obtained for such a diverse group of molecules (48 classes involving 2924 data points) demonstrates the validity of this integrated approach and provides credible evidence to support the above hypothesis.

Conclusions

1. Our SVRC framework successfully correlated STs of a diverse subset of organic molecules over a wide temperature range in the saturation region. The SVRC model was able to represent STs of 198 molecules with an AAD of 0.6% on average when one adjustable parameter was used for each substance.
2. The SVRC-QSPR models provide excellent generalized predictions of STs, with average errors of less than 1.2%, based on structural descriptors and end-point input data.
3. The generalized SVRC-QSPR model was capable of making *a priori* predictions for the compounds in the external database with an overall AAD of ~6%.
4. The results of this study indicate that the use of theory-framed structure-property modeling is effective in thermo-physical model generalization.
5. The limited database employed in the present work constrained the model generalization efforts. These results, however, constitute a promising initial effort in our quest to develop a robust and effective model based on a larger database.

Recommendations

1. Assemble a larger database of experimental measurements involving more diverse molecular species. Availability of such data would facilitate better training of the neural network, which, in turn, would lead to the development of a more robust model capable of being extensively validated.
2. Develop a generalized QSPR model for predicting surface tensions at the triple point temperatures to serve as input data for the generalized SVRC-QSPR model.

References

1. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Vapor Pressures. Fluid Phase Equilibria, 1991. 64: p. 141-163.

2. Shaver, R.D., R.L. Robinson, Jr., and K.A.M. Gasem, A Framework for the Prediction of Saturation Properties: Liquid Density. Fluid Phase Equilibria, 1992. 64: p. 81-98.

3. Godavarthy, S., R.L. Robinson, Jr., and K.A.M. Gasem, SVRC-QSPR Model for Predicting Saturated Vapor Pressures of Pure Fluids. Fluid Phase Equilibria, Volume 246, Issues 1-2, 25 August 2006, Pages 39-51.

4. Reid, R.C., et al., The Properties of Gases and Liquids. 1987, New York: McGraw-Hill.

5. Fanchl, J.R., Calculation of parachors for compositional simulation. An update. SPE Reservoir Engineering, 1990. v 5(n 3): p. p 433-436.

6. Ali, J.K., Prediction of Parachors of Petroleum Cuts and Pseudocomponents. Fluid Phase Equilibria, 1995. 95: p. 383-398.

7. Schechter, D.S.G., B. Parachors Based on Modern Physics and Their Uses in IFT Prediction of Reservoir Fluids. in Proceedings - SPE Annual Technical Conference and Exhibition. 1995. Dallas, TX, USA: Society of Petroleum Engineers (SPE), Richardson, TX, USA.

8. Broseta, D.R., Karine. Parachors in Terms of Critical Temperature, Critical Pressure and Acentric Factor. in Proceedings of the 1995 SPE Annual Technical Conference and Exhibition. 1995. Dallas, TX, USA.

9. Zuo, Y.-X.S., E.H., Corresponding-States and Parachor Models for the Calculation of Interfacial Tensions. Canadian Journal of Chemical Engineering, 1997. v 75(n 6): p. 1130-1137.

10. Cumber, P., Surface Tension Prediction for Hydrocarbons and its Application to Level Swell Modeling. Journal of Hazardous Materials, 2002. A 89: p. 127-139.

11. Gasem, K.A.M., et al., Test of prediction Methods for Interfacial Tensions of CO_2 and Ethane in Hydrocarbon Solvents. Fluid Phase Equilibria, 1989. 53: p. 39-50.

12. Dandekar, A.Y., Sensitivity Analysis of Interfacial Tension Predictions for Hydrocarbon Fluids. Petroleum Science and Technology, 2004. v 22 (n 9-10): p. 1161-1172.

13. Lu, J.-F., et al., Application of Density Functional Theory for Predicting the Surface Tension of Pure Polar and Associating Fluids. Fluid Phase Equilibria, 2002. 194-197: p. 755-769.

14. Do, D.D., E. Ustinov, and H.D. Do, Phase Equilibria and Surface Tension of Pure Fluids Using a Molecular Layer Structure Theory (MLST) Model. Fluid Phase Equilibria, 2003. 204: p. 309-326.

15. Espósito, R.O., F.W. Tavares, and M. Castier, Phase Equilibrium Calculations for Confined Fluids, Including Surface Tension Prediction Models. Brazilian Journal of Chemical Engineering, 2005. 22(1): p. 93-104.

16. Egemen, E., N. Nirmalakhandan, and C. Trevizo, Predicting Surface Tension of Liquid Organic Solvents. Environ. Sci. Technol., 2000. 34: p. 2596-2600.

17. Kauffman, G.W. and P.C. Jurs, Prediction of Surface Tension, Viscosity, and Thermal Conductivity for Common Organic Solvents Using Quantitative Structure-Property Relationships. J. Chem. Inf. Comput. Sci., 2001. 41: p. 408-418.

18. Knotts, T.A., et al., Use of the DIPPR Database for Development of QSPR Correlations: Surface Tension. J. Chem. Eng. Data, 2001. 46: p. 1007-1012.

19. S. S. Godavarthy, Design of Improved Solvents for Extractive Distillation, Oklahoma State University, Ph.D. Dissertation, 2004.

20. Project 801, Physical and Thermodynamic Property Database. 1999, Design Institute for Physical Property Data.

21. Jasper, J.J., The Surface Tension of Pure Liquid Compounds. Journal of Physical and Chemical Reference Data, 1972. 1: p. 841.

22. ChemDraw 8.0. 2004, Cambridge Software.

23. AMPAC 6.0. 1997, Semichem Inc.

24. CODESSA 2.63. 1998, Semichem Inc.

25. Yaffe, D.L., A Neural Network Approach for Estimating Physicochemical Properties Using Quantitative Structure-Property Relationships (QSPRs), University of California: Los Angeles, Ph.D. Thesis, 2001.

26. Ravindranath, D., Structure-Based Generalized Models for Pure-Fluid Saturation Properties and Activity Coefficients, Oklahoma State University: Stillwater, M.S. Thesis, 2005

27. Mitchell, B. and C.P. Jurs, Prediction of Autoignition Temperatures of Organic Compounds from Molecular Structure. J. Chem. Inf. Comput. Sci, 1997. 37: p. 538-547.

28. Wessel, M.D., J.M. Sutter, and C.P. Jurs, Prediction of Reduced Ion Mobility Constants of Organic Compounds from Molecular Structure. Anal. Chem, 1996. 68: p. 4237-4243.

29. Venkatasubramanian, V., K. Chan, and J.M. Caruthers, Computer-Aided Molecular Design Using Genetic Algorithms. Computers Chem. Engng, 1994. 18(9): p. 833-844.

30. Mitchell, B. and C.P. Jurs, Prediction of Infinite Dilution Activity Coefficients of Organic Compounds in Aqueous Solution from Molecular Structure. J. Chem. Inf. Comput. Sci., 1998. 38: p. 200-209.

31. Wessel, M.D., et al., Prediction of Human Intestinal Absorption of Drug Compounds from Molecular Structure. Molecular Modeling and Prediction of Bioavailability, 2000: p. 249-255.

32. Randic, M., Orthogonal Molecular Descriptors. New J. Chem, 1991. 15: p. 517-525.

33. Lucic, B., et al., The Structure-Property Models Can Be Improved Using the Orthogonalized Descriptors. J. Chem. Inf Comput. Sci., 1995. 35: p. 532-538.

34. NeuralWare, Predict 3.10. Feb 2003: Carnegie, PA15106-2700.

35. Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Gases and Liquids. 4 ed. 1987: McGraw Hill.

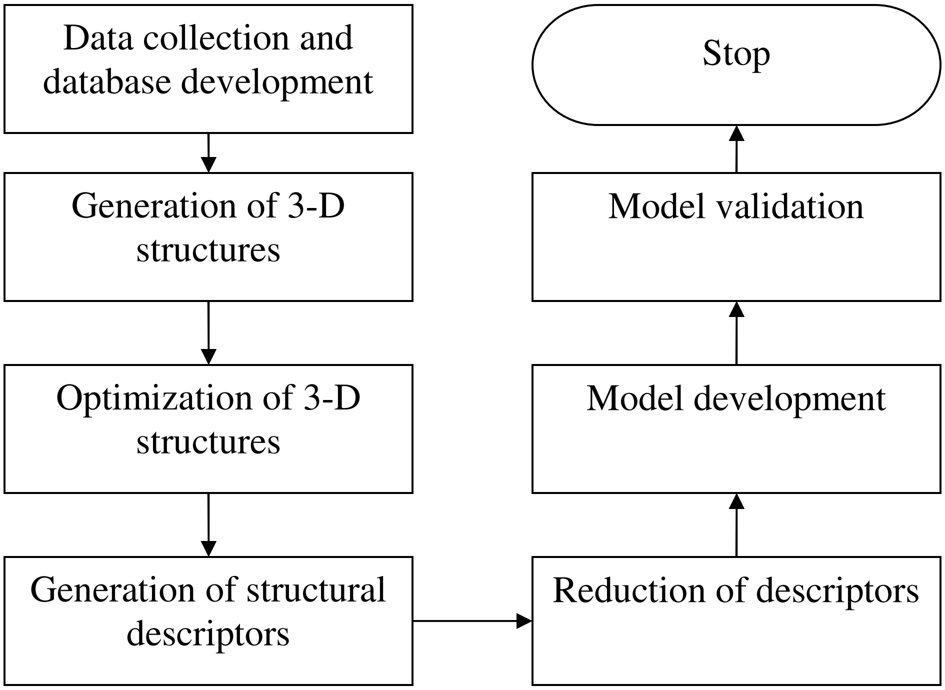

Figure 4.1. Overview of QSPR Methodology [20]

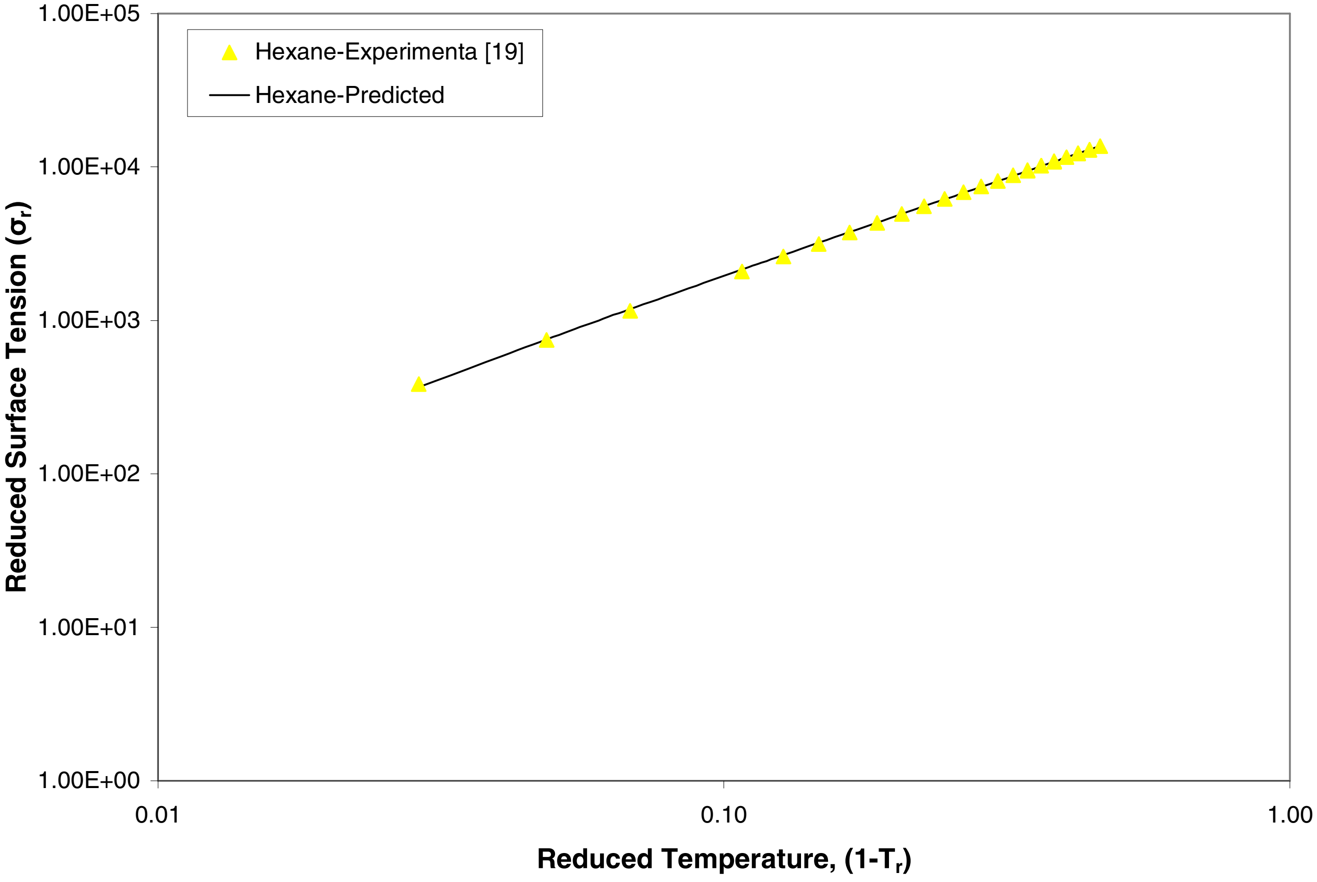

Figure 4.2. Variation of reduced surface tension with temperature

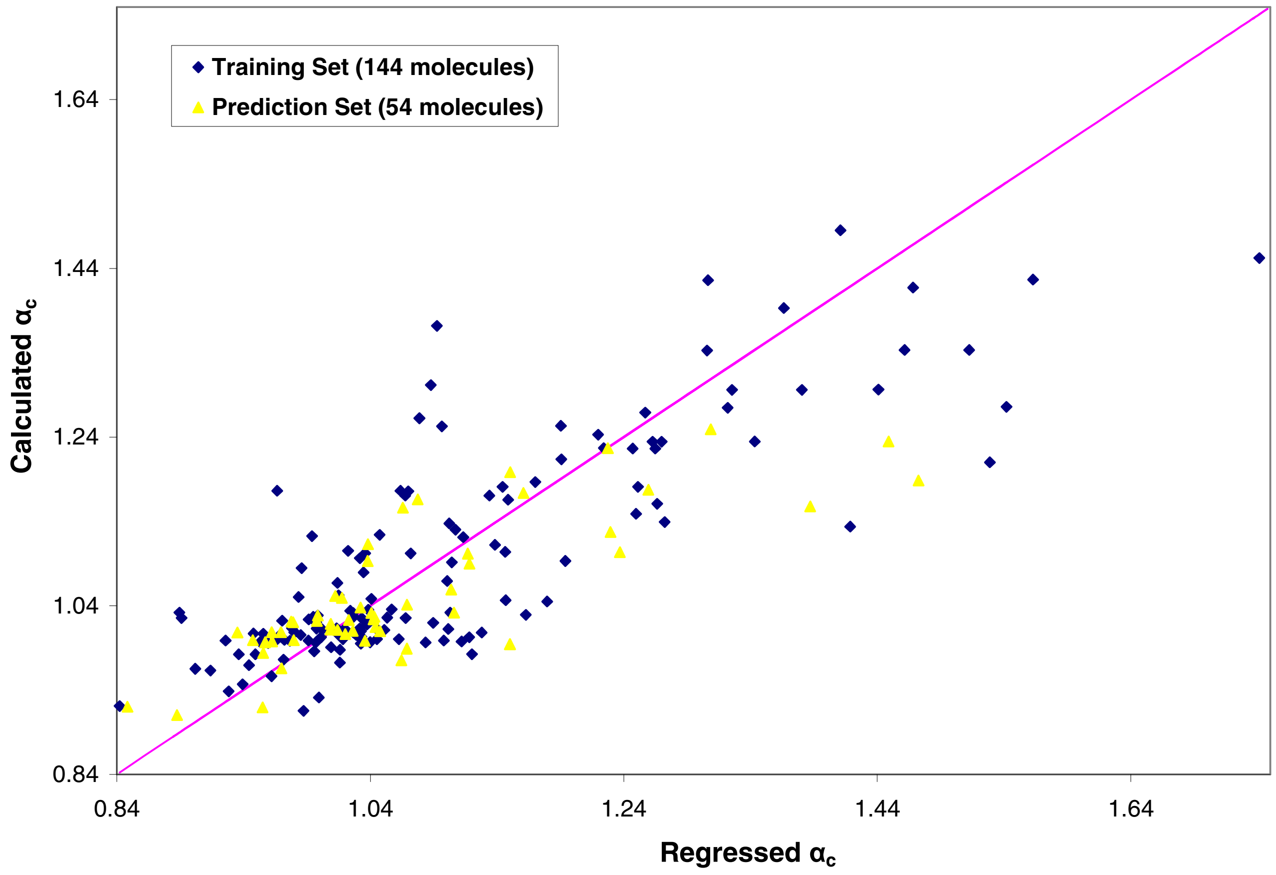

Figure 4.3. Comparison of regressed α_c and calculated α_c of the SVRC-QSPR model for surface tension

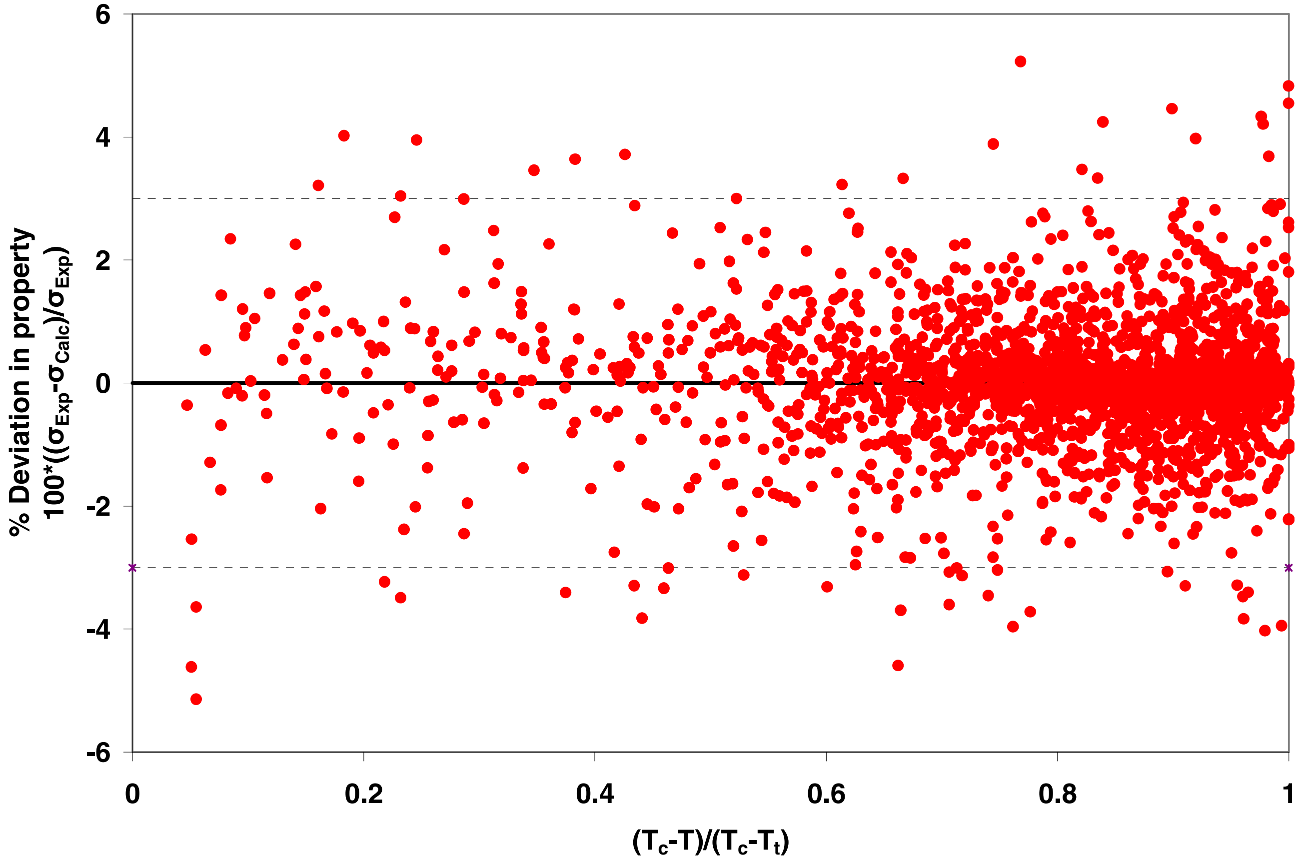

Figure 4.4. Deviations in regressed surface tensions using the SVRC model

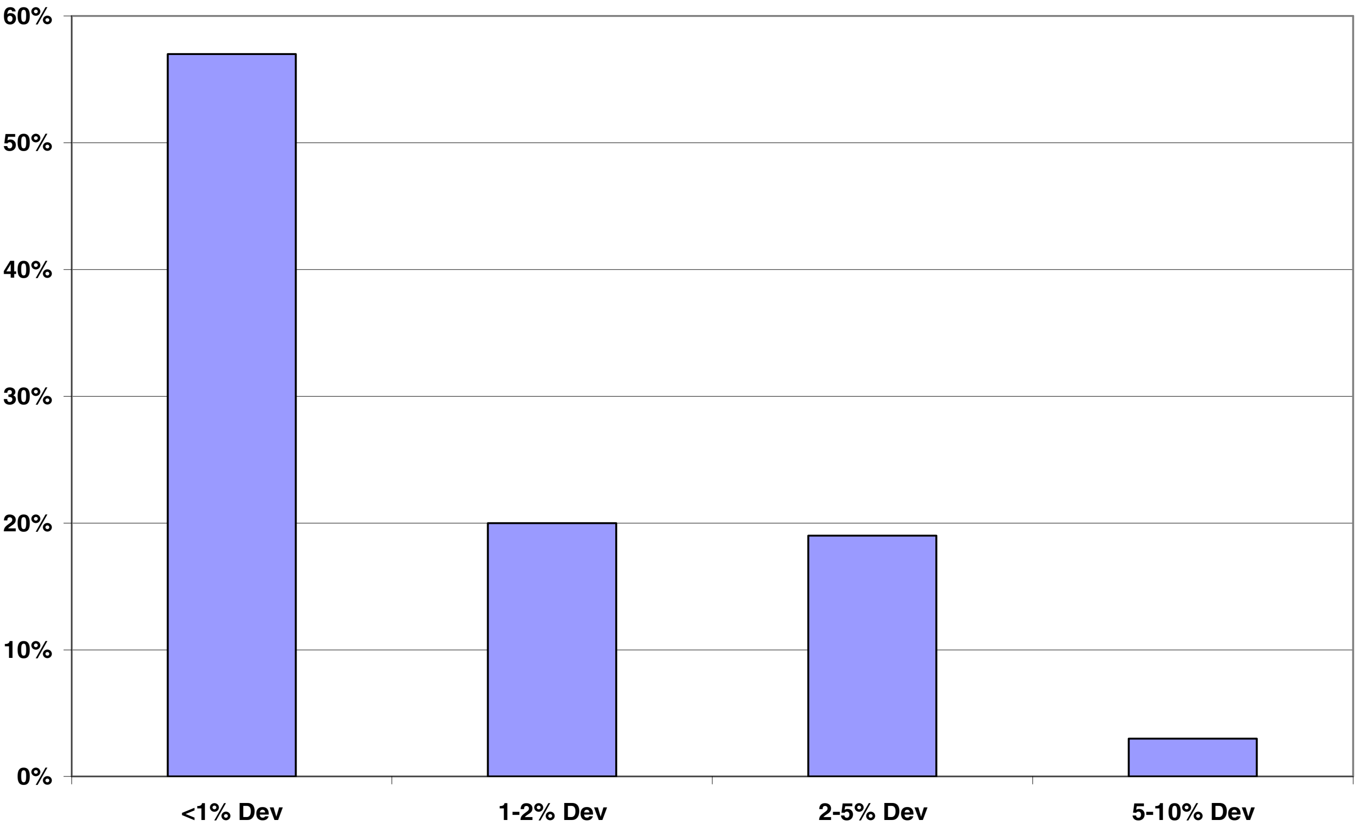

Figure 4.5. Distribution of errors (deviations) in predicted surface tensions using the generalized SVRC-QSPR model

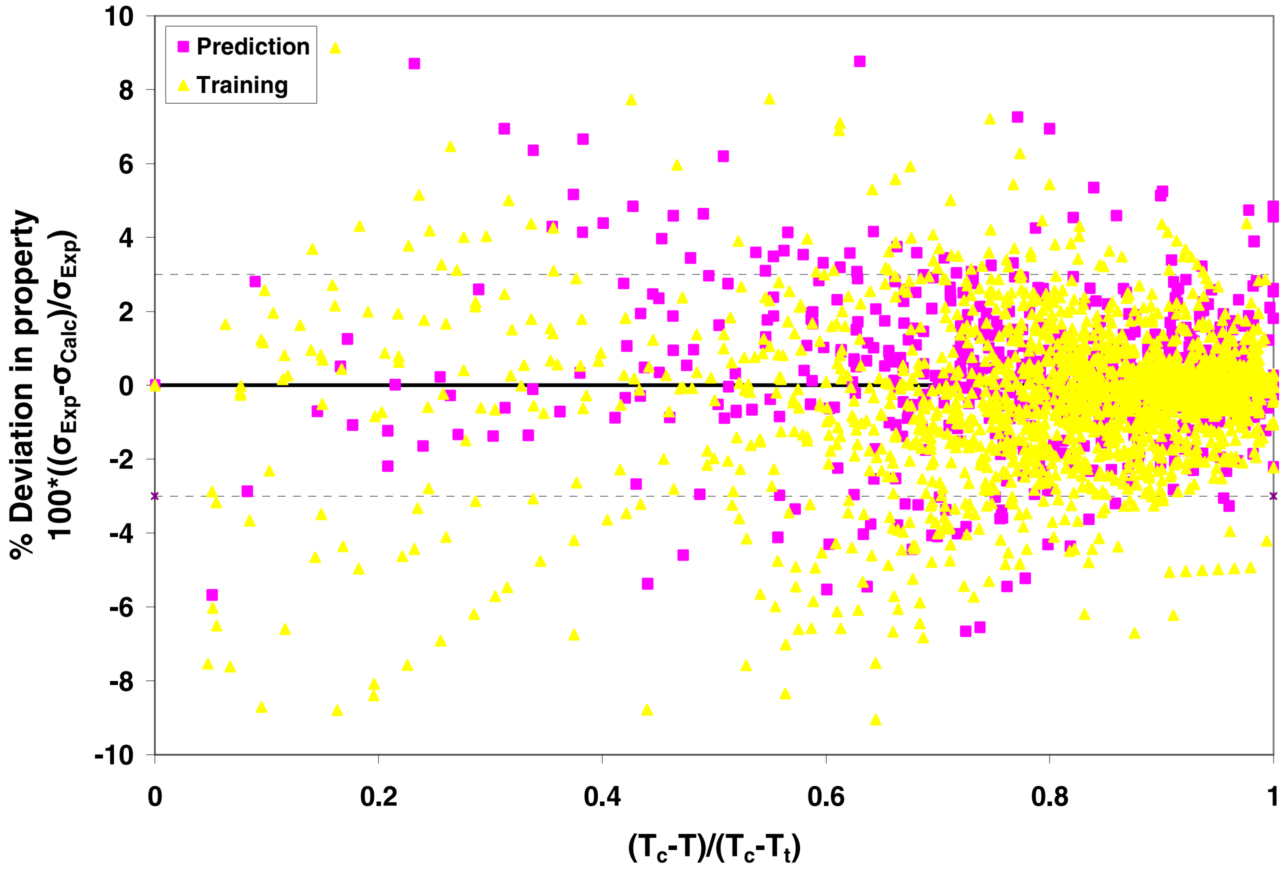

Figure4.6. Deviations in predicted surface tensions using the generalized SVRC-QSPR model

.

Table 4.1. Summary of results using regressed and predicted SVRC Model Parameters

Chemical Class	Case 1: %AAD of SVRC Model Regressions	Case 2: %AAD of Generalized SVRC-QSPR Model	Datasets
SULFIDES/THIOPHENES	1.08	1.19	02
SILANES/SILOXANES	0.72	0.85	08
PROPIONATES AND BUTYRATES	0.66	0.76	05
POLYFUNCTIONAL C, H, O, N	0.33	0.43	03
POLYFUNCTIONAL C, H, O, HALIDE	0.32	0.66	01
POLYFUNCTIONAL C, H, N, HALIDE, (O)	0.28	1.23	02
POLYFUNCTIONAL AMIDES/AMINES	0.17	0.30	01
OTHER SATURATED ALIPHATIC ESTERS	0.39	1.01	03
OTHER POLYFUNCTIONAL C, H, O	1.15	1.77	03
OTHER INORGANICS	1.44	1.44	01
OTHER ETHERS/DIETHERS	1.40	2.07	04
OTHER ALKYLBENZENES	0.72	1.18	15
OTHER ALIPHATIC AMINES	0.44	0.56	01
OTHER ALIPHATIC ALCOHOLS	0.70	1.26	10
OTHER ALIPHATIC ACIDS	0.79	2.87	01
ORGANIC SALTS	0.53	1.54	03
NITRILES	0.44	0.85	02
N-ALKYLBENZENES	0.39	1.06	05
N-ALKANES	0.41	1.10	08
N-ALIPHATIC PRIMARY AMINES	1.54	4.76	01
N-ALIPHATIC ACIDS	0.75	2.27	04
N-ALCOHOLS	0.48	1.28	11
MULTIRING CYCLOALKANES	0.58	0.89	02
METHYLALKENES	0.75	0.75	01
METHYLALKANES	0.74	1.39	06

Table 4.1. Summary of results using regressed and predicted SVRC Model Parameters (contd.)

Chemical Class	Case 1: %AAD of SVRC Model Regressions	Case 2: %AAD of Generalized SVRC-QSPR Model	Datasets
KETONES	0.63	1.42	09
INORGANIC GASES	0.87	1.69	02
FORMATES	0.73	1.25	06
EPOXIDES	0.15	0.73	02
ELEMENTS	0.45	0.45	01
DIPHENYL/POLYAROMATICS	0.84	1.27	05
DIMETHYLALKANES	0.22	0.87	01
CYCLOALKENES	0.38	0.83	02
C3 & HIGHER ALIPHATIC CHLORIDES	0.46	0.64	02
C,H,F COMPOUNDS	0.63	0.88	06
C, H, NO2 COMPOUNDS	0.61	1.13	07
C, H, MULTIHALOGEN COMPOUNDS	0.43	1.01	06
C, H, I COMPOUNDS	0.58	0.77	02
C, H, F COMPOUNDS	0.71	1.39	04
AROMATIC ESTERS	0.83	0.94	03
AROMATIC CHLORIDES	0.32	0.50	01
AROMATIC AMINES	0.63	1.20	07
AROMATIC ALCOHOLS	0.65	0.81	01
ANHYDRIDES	0.63	1.46	02
ALIPHATIC ETHERS	0.46	1.23	03
ALDEHYDES	0.27	1.77	03
ACETATES	0.49	1.23	10
OTHER ALIPHATIC AMINES	0.90	1.30	01
1-ALKENES	0.40	1.23	08
OTHER SATURATED ALIPHATIC ESTERS	1.60	1.87	01
Overall %AAD	**0.6**	**1.2**	

Table 4.2. Descriptors obtained from non-linear modeling of the model parameter α_c

Descriptors
Gravitation index (all bonds)
Average Information content (order 2)
Average Bonding Information content (order 2)
HA dependent HDSA-2 [Zefirov's PC]
HA dependent HDSA-2/SQRT(TMSA) [Zefirov's PC]
HACA-2 [Zefirov's PC]
HOMO-1 energy
FHACA Fractional HACA (HACA/TMSA) [Quantum-Chemical PC]
HA dependent HDSA-2/TMSA [Quantum-Chemical PC]
Max nucleoph. react. index for a O atom
PPSA-2 Total charge weighted PPSA [Quantum-Chemical PC]
Min resonance energy for a C-S bond

Table 4.3. Results of secondary validation for the generalized SVRC-QSPR model using an external dataset

Chemical classes represented in the training set	%AAD	Datasets
1-ALKENES	1.3	19
ACETATES	2.0	11
ALDEHYDES	4.2	32
ANHYDRIDES	3.2	15
AROMATIC ESTERS	10.0	4
CYCLOALKENES	7.0	9
DIMETHYLALKANES	6.7	16
DIPHENYL/POLYAROMATICS	6.1	18
ELEMENTS	4.7	6
FORMATES	5.7	10
INORGANIC GASES	5.0	8
KETONES	6.5	23
METHYLALKANES	7.6	17
METHYLALKENES	7.6	16
MULTIRING CYCLOALKANES	1.4	3
N-ALCOHOLS	7.7	20
N-ALIPHATIC ACIDS	6.7	15
N-ALKANES	6.5	29
N-ALKYLBENZENES	7.5	15
OTHER ALIPHATIC ACIDS	6.4	16
OTHER ALIPHATIC ALCOHOLS	6.8	30
OTHER ALKANES	7.2	22
OTHER ALKYLBENZENES	6.1	35
OTHER ETHERS/DIETHERS	2.8	2
OTHER MONOAROMATICS	6.0	19
OTHER POLYFUNCTIONAL C, H, O	3.3	3
OTHER SATURATED ALIPHATIC ESTERS	2.5	7
PROPIONATES AND BUTYRATES	4.6	9

Table 4.4. Results of secondary validation for the generalized SVRC-QSPR model using an external dataset

Chemical classes not represented in the training set	%AAD	Datasets
2,3,4-ALKENES	1.5	19
ALKYLCYCLOHEXANES	3.9	16
ALKYLCYCLOPENTANES	3.3	10
ALKYNES	3.2	7
AROMATIC ALCOHOLS	3.4	5
AROMATIC CARBOXYLIC ACIDS	6.8	4
CYCLOALIPHATIC ALCOHOLS	7.7	10
CYCLOALKANES	9.9	6
DIALKENES	5.7	26
DICARBOXYLIC ACIDS	7.0	4
ETHYL & HIGHER ALKENES	7.1	12
NAPHTHALENES	6.0	15
OTHER CONDENSED RINGS	6.3	10
OTHER HYDROCARBON RINGS	6.0	16
POLYFUNCTIONAL ACIDS	6.6	2
POLYFUNCTIONAL C, H, O, N	13.7	2
POLYOLS	6.5	35
TERPENES	4.9	8
UNSATURATED ALIPHATIC ESTERS	5.4	6
2,3,4-ALKENES	4.9	16
ALKYLCYCLOHEXANES	1.8	14
ALKYLCYCLOPENTANES	2.3	12
ALKYNES	3.6	13
AROMATIC CARBOXYLIC ACIDS	3.2	9
AROMATIC CHLORIDES	4.1	10
C, H, BR COMPOUNDS	3.2	14
C1/C2 ALIPHATIC CHLORIDES	2.9	18
CYCLOALIPHATIC ALCOHOLS	3.2	8
CYCLOALKANES	1.8	4
DIALKENES	7.3	23
DICARBOXYLIC ACIDS	3.7	13
ETHYL & HIGHER ALKENES	2.9	12
INORGANIC ACIDS	6.9	5
INORGANIC BASES	4.3	1
INORGANIC HALIDES	9.5	11
ISOCYANATES/DIISOCYANATES	6.4	3
MERCAPTANS	3.2	14
NAPHTHALENES	5.4	15
NITROAMINES	1.5	4
ORGANIC/INORGANIC COMPOUNDS	5.9	3
OTHER AMINES, IMINES	4.3	31
OTHER CONDENSED RINGS	3.9	8

Table 4.4. Results of secondary validation for the generalized SVRC-QSPR model using an external dataset (contd.)

Chemical classes not represented in the training set	%AAD	Datasets
OTHER HYDROCARBON RINGS	3.8	12
OTHER MONOAROMATICS	8.1	14
OTHER POLYFUNCTIONAL ORGANICS	11.8	4
PEROXIDES	2.0	10
POLYFUNCTIONAL ACIDS	4.5	19
POLYFUNCTIONAL C, H, N, HALIDE, (O)	5.6	9
POLYFUNCTIONAL C, H, O, N	5.3	19
POLYFUNCTIONAL C, H, O, S	7.8	11
POLYFUNCTIONAL ESTERS	5.0	18
POLYOLS	9.1	22
TERPENES	5.5	8
UNSATURATED ALIPHATIC ESTERS	3.8	19

APPENDIX A

THE SVRC-QSPR MODEL FOR LIQUID VISCOSITIES: DATABASE USED FOR MODEL DEVELOPMENT AND VALIDATION

Table A.1. Liquid viscosity data used in model development [1]

Compound	Reduced Temperature Range	Data Points	Classification
3-METHYLPENTANE	0.53-0.66	11	PR
2-METHYLHEXANE	0.52-0.69	25	PR
DODECANE	0.40-0.65	24	TR
TRIDECANE	0.40-0.70	16	TR
TETRADECANE	0.40-0.61	23	TR
HEXADECANE	0.41-0.78	10	TR
HEPTADECANE	0.40-0.78	11	TR
METHYLCYCLOPENTANE	0.47-0.66	30	TR
ETHYLCYCLOPENTANE	0.44-0.66	28	TR
BUTYLCYCLOHEXANE	0.38-0.57	8	PR
cis-DECALIN	0.35-0.64	27	TR
trans-DECALIN	0.35-0.66	20	TR
1-DECENE	0.44-0.67	22	TR
1-HEXADECENE	0.38-0.52	9	TR
BENZENE, 1,3-DIMETHYL-	0.44-0.58	12	PR
BENZENE,BUTYL	0.42-0.55	13	TR
BENZENE,DECYL	0.34-0.56	31	TR
BIPHENYL	0.45-0.94	27	TR
1,1':4', 1"-TERPHENYL	0.53-0.80	22	TR
BENZENE,PENTYL	0.42-0.55	11	PR
BENZENE,HEXYL	0.36-0.61	24	TR
BENZENE,NONYL	0.34-0.54	25	TR
BENZENE,TETRADECYL	0.35-0.47	10	TR
BENZENE,ETHENYL	0.43-0.66	17	TR
NAPHTHALENE, 1-METHYL-	0.35-0.48	9	PR
NAPHTHALENE, 2-METHYL-	0.41-0.49	18	TR
BENZALDEHYDE, 2-HYDROXY-	0.44-0.69	16	TR
TRIOXANE,2,4,6-TRIMETHYL	0.49-0.67	13	TR
2-BUTANONE	0.42-0.66	13	TR
3-PENTANONE	0.49-0.66	19	PR
2-PENTANONE	0.49-0.66	26	TR
2-PYROLIDINONE	0.37-0.46	14	TR
CYCLOPENTANONE	0.47-0.58	18	PR
ETHANONE, 1-PHENYL-	0.42-0.52	19	PR
1-HEXANOL	0.46-0.70	16	TR
2-HEXANOL	0.48-0.70	13	TR
1-PENTANOL, 2-METHYL-	0.46-0.68	15	PR
1-BUTANOL, 3-METHYL-	0.47-0.70	19	PR
1-HEPTANOL	0.46-0.71	8	TR
2-PENTANOL, 4-METHYL-	0.49-0.69	15	TR
1-OCTANOL	0.44-0.56	14	TR

Table A.1. Liquid viscosity data used in model development

Compound	Reduced Temperature Range	Data Points	Classification
1-HEXADECANOL	0.42-0.74	14	TR
CYCLOHEXANOL	0.46-0.66	8	TR
2-PROPEN-1-OL	0.52-0.68	19	TR
1,2-BENZENEDIOL	0.50-0.66	13	TR
FORMIC ACID	0.48-0.64	18	TR
PROPANOIC ACID	0.47-0.60	18	TR
PROPANOIC ACID, 2-METHYL-	0.45-0.70	34	TR
HEXANOIC ACID	0.44-0.56	27	TR
DODECANOIC ACID	0.44-0.58	10	TR
OCTADECANOIC ACID	0.43-0.59	9	TR
ACETIC ACID, ANHYDRIDE	0.45-0.67	19	TR
PROPANOIC ACID, ANHYDRIDE	0.44-0.70	24	TR
FORMIC ACID, PROPYL ESTER	0.51-0.66	18	TR
ACETIC ACID, METHYL ESTER	0.54-0.82	38	TR
ACETIC ACID, BUTYL ESTER	0.50-0.60	21	TR
1-BUTANOL, 3-METHYL-	0.48-0.79	13	TR
PROPANOIC ACID	0.51-0.66	20	PR
PROPANOIC ACID, 2-METHYL-	0.50-0.67	13	PR
BUTANOIC ACID, ETHYL ESTER	0.51-0.60	11	PR
BENZOIC ACID,2-HYDROXY,METHYL ESTER	0.42-0.70	6	TR
BENZOIC ACID, ETHYL ESTER	0.41-0.49	12	TR
CARBONIC ACID, DIETHYL ESTER	0.49-0.68	22	TR
ETHANEDIOIC ACID, DIETHYL ESTER	0.44-0.70	13	TR
PROPANEDIOIC ACID, DIETHYL ESTER	0.44-0.46	11	TR
PROPANE, 1-ETHOXY-	0.55-0.67	12	TR
1,4-DIOXANE	0.49-0.64	20	PR
PROPANE, 1,1'-OXYBIS-	0.29-0.68	15	TR
ETHANE, 1,2-DIMETHOXY-	0.38-0.56	9	PR
BENZENE, ETHOXY-	0.42-0.69	22	TR
FURAN, TETRAHYDRO-	0.38-0.64	25	TR
2-FURANMETHANOL	0.47-0.64	8	TR
ETHANE,2DIFLUOROMETHOXYTRIFl	0.56-0.75	20	PR
BENZENE, 1-CHLORO-3-NITRO-	0.43-0.57	18	TR
BENZENEACETONITRILE	0.40-0.65	10	TR
1,2-ETHANEDIOL, NITRATE	0.43-0.51	12	TR
PHENOL, 2-METHOXY-	0.46-0.69	13	TR
ACETALDEHYDE, TRICHLORO-	0.52-0.66	12	TR

Table A2. Liquid viscosity data used for external validation

Compound Name	Reduced Temperature Range	%AAD	Data points
METHANE	0.46-1.00	24.7	59
ETHANE	0.30-1.00	39.9	136
PROPANE	0.23-1.00	44.1	155
PROPANE, 2-METHYL-	0.28-0.98	39.9	73
BUTANE	0.31-1.00	37.7	126
BUTANE, 2-METHYL-	0.49-0.66	0.3	12
PROPANE, 2,2-DIMETHYL-	0.60-0.70	0.4	13
HEXANE	0.34-1.00	31.9	115
PENTANE, 2-METHYL-	0.24-0.67	10.9	31
PENTANE, 3-METHYL-	0.53-0.66	0.7	11
BUTANE, 2,2-DIMETHYL-	0.55-0.66	1.9	10
BUTANE, 2,3-DIMETHYL-	0.55-0.63	6.8	13
HEPTANE	0.33-1.00	32.2	122
HEXANE, 2-METHYL-	0.29-0.69	5.0	39
HEXANE, 3-METHYL-	0.29-0.68	7.5	18
PENTANE, 3-ETHYL-	0.29-0.67	8.0	12
PENTANE, 2,2-DIMETHYL-	0.29-0.79	30.3	24
PENTANE, 2,3-DIMETHYL-	0.28-0.67	12.5	17
PENTANE, 2,4-DIMETHYL-	0.33-0.66	4.8	16
PENTANE, 3,3-DIMETHYL-	0.26-0.67	18.2	12
BUTANE, 2,2,3-TRIMETHYL-	0.47-0.67	1.0	13
OCTANE	0.37-1.00	28.2	135
HEPTANE, 2-METHYL-	0.29-0.97	40.2	23
HEPTANE, 3-METHYL-	0.27-0.68	12.4	14
HEPTANE, 4-METHYL-	0.27-0.68	12.4	14
HEXANE, 3-ETHYL-	0.48-0.68	0.4	14
HEXANE, 2,2-DIMETHYL-	0.28-0.68	16.7	14
HEXANE, 2,3-DIMETHYL-	0.48-0.68	4.9	14
HEXANE, 2,4-DIMETHYL-	0.49-0.69	0.3	11
HEXANE, 2,5-DIMETHYL-	0.33-0.70	9.6	16
HEXANE, 3,3-DIMETHYL-	0.26-0.67	16.4	14
HEXANE, 3,4-DIMETHYL-	0.48-0.67	5.1	14
PENTANE, 3-ETHYL-2-METHYL-	0.28-0.69	11.2	11
PENTANE, 3-ETHYL-3-METHYL-	0.32-0.66	6.1	14
PENTANE, 2,2,3,TRIMETHYL-	0.29-0.68	13.4	23
PENTANE, 2,2,4-TRIMETHYL-	0.32-1.00	62.1	54
PENTANE, 2,3,3-TRIMETHYL-	0.30-0.79	25.7	14
PENTANE, 2,3,4-TRIMETHYL-	0.29-0.78	15.4	14

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BUTANE, 2,2,3,3-TETRAMETHYL-	0.52-0.80	17.8	22
NONANE	0.37-1.00	32.2	112
HEXANE, 2,2,5-TRIMETHYL-	0.29-0.68	4.9	11
HEPTANE, 3,3,5-TRIMETHYL-	0.27-0.80	33.8	11
HEXANE,2,4,4-TRIMETHYL-	0.28-0.79	36.2	21
PENTANE, 3,3-DIETHYL-	0.39-0.67	0.6	11
PENTANE, 2,2,3,3,-TETRAMETHYL-	0.43-0.80	9.7	10
PENTANE, 2,2,3,4-TETRAMETHYL-	0.26-0.80	35.1	10
PENTANE, 2,2,4,4-TETRAMETHYL-	0.36-0.80	22.1	10
PENTANE, 2,3,3,4-TETRAMETHYL-	0.28-0.80	33.7	20
TETRACOSANE, 2,6,10,15,19,23-HEXAMETHYL-	0.25-0.61	69.6	36
DECANE	0.39-0.99	26.8	145
HEXANE, 2,2,5,5-TETRAMETHYL-	0.45-0.80	10.6	10
UNDECANE	0.39-1.01	30.4	122
DODECANE	0.40-1.00	29.2	152
TRIDECANE	0.40-1.01	29.6	195
TETRADECANE	0.40-0.99	27.4	200
PENTADECANE	0.40-0.99	31.4	187
HEXADECANE	0.40-0.99	29.9	199
HEPTADECANE	0.40-0.98	27.9	173
OCTADECANE	0.40-0.98	32.0	163
NONADECANE	0.40-0.98	35.2	192
OCTANE, 2,2-DIMETHYL-	0.37-0.71	3.7	11
EICOSANE	0.40-0.98	34.9	220
HENEICOSANE	0.40-0.81	5.5	19
DOCOSANE	0.40-0.97	31.5	28
TRICOSANE	0.40-0.82	6.4	23
TETRACOSANE	0.41-0.99	23.7	12
PENTACOSANE	0.40-0.84	6.5	16
HEXACOSANE	0.40-0.99	30.2	36
HEPTACOSANE	0.40-0.84	5.3	11
OCTACOSANE	0.40-1.00	27.5	26
NONACOSANE	0.40-0.85	6.0	11
NONANE, 3-METHYL-	0.31-0.72	10.1	14
NONANE, 2-METHYL-	0.33-0.97	40.6	53
NONANE, 4-METHYL-	0.29-0.71	14.1	14
NONANE, 5-METHYL	0.30-0.71	10.3	14
OCTANE, 2-METHYL-	0.33-0.98	37.4	22
OCTANE, 3-METHYL-	0.28-0.70	12.3	11

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
OCTANE, 4-METHYL-	0.27-0.70	14.4	11
3-ETHYLHEPTANE	0.27-0.69	27.5	13
HEPTANE, 2,2-DIMETHYL-	0.28-0.69	18.1	11
UNDECANE, 3-METHYL-	0.33-0.74	7.5	10
CYCLOPROPANE	0.37-0.80	2.1	10
CYCLOBUTANE	0.40-0.80	0.7	10
CYCLOPENTANE	0.49-0.63	0.8	13
CYCLOPENTANE, METHYL-	0.47-0.66	2.1	45
CYCLOPENTANE, ETHYL-	0.45-0.66	0.4	46
CYCLOPENTANE, 1,1-DIMETHYL-	0.37-0.65	0.5	11
CYCLOPENTANE, 1,2-DIMETHYL-, cis-	0.39-0.80	13.8	22
CYCLOPENTANE, 1,2-DIMETHYL-, trans-	0.28-0.79	32.4	22
CYCLOPENTANE, 1,3-DIMETHYL-, cis-	0.25-0.65	13.5	11
CYCLOPENTANE, 1,3-DIMETHYL-, trans-	0.25-0.65	13.8	11
CYCLOPENTANE, PROPYL-	0.43-0.64	2.2	33
CYCLOPENTANE,(1-METHYLETHYL)-	0.27-0.67	12.0	13
CYCLOPENTANE, 1-ETHYL-1-METHYL-	0.22-0.67	25.4	11
CYCLOPENTANE, 1-BUTYL-	0.27-0.69	18.1	25
CYCLOHEXANE	0.50-1.00	18.3	87
CYCLOHEXANE, METHYL-	0.37-0.69	8.4	74
CYCLOHEXANE, ETHYL-	0.41-0.63	1.5	36
CYCLOHEXANE, 1,1-DIMETHYL-	0.41-0.66	0.6	11
CYCLOHEXANE, 1,2-DIMETHYL-, cis-	0.37-0.65	15.8	43
CYCLOHEXANE, 1,2-DIMETHYL-, trans-	0.31-0.66	7.3	16
CYCLOHEXANE, 1,3-DIMETHYL-, cis-	0.33-0.66	5.2	16
CYCLOHEXANE, 1,3-DIMETHYL-, trans-	0.31-0.66	7.1	32
CYCLOHEXANE, 1,4-DIMETHYL-, cis-	0.31-0.66	8.4	16
CYCLOHEXANE, 1,4-DIMETHYL-, trans-	0.40-0.67	5.8	34
CYCLOHEXANE, 1,3,5-TRIMETHYL-, trans	0.31-0.69	10.7	11
CYCLOHEXANE, PROPYL-	0.39-0.60	3.3	35
CYCLOHEXANE, (1-METHYL ETHYL)-	0.29-0.68	14.9	14
CYCLOHEXANE,-1,2,3,4-TETRAMETHYL-	0.31-0.70	12.8	10

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
CYCLOHEXANE, BUTYL-	0.38-0.80	8.3	36
cis-DECALIN	0.35-0.64	1.8	54
trans-DECALIN	0.35-0.66	1.1	54
1,1'-BICYCLOHEXYL	0.40-0.42	0.5	5
CYCLOHEXANE, 1,1-DIETHYL-	0.27-0.74	17.5	16
CYCLOHEXANE, DECYL-	0.36-0.43	3.2	12
CYCLOHEPTANE	0.44-0.80	1.0	11
CYCLOOCTANE	0.44-0.80	8.7	20
CYCLOHEXANE, trans-1,4-DIETHYL	0.48-0.48	0.0	1
HEPTANE, 2,6-DIMETHYL-	0.29-0.69	14.5	11
3-ETHYLPENTANE, 2-2-DIMETHYL-	0.29-0.68	12.8	11
3-ETHYLPENTANE, 2,4-DIMETHYL-	0.26-0.68	22.4	11
ETHENE	0.37-0.99	30.7	44
1-PROPENE	0.24-0.99	32.3	31
1-BUTENE	0.40-0.57	0.8	9
2-BUTENE, (Z)-	0.31-0.77	6.0	18
2-BUTENE, (E)-	0.39-0.78	5.5	18
1-PROPENE, 2-METHYL-	0.32-0.82	10.2	21
1-PENTENE	0.39-0.59	0.6	11
2-PENTENE, (Z)-	0.26-0.65	2.2	11
2-PENTENE, (E)-	0.28-0.65	1.2	11
1-BUTENE, 2-METHYL-	0.29-0.64	1.4	11
1-BUTENE, 3-METHYL-	0.60-0.68	1.7	10
2-BUTENE, 2-METHYL-	0.30-0.66	3.0	19
1-HEXENE	0.43-0.66	3.7	20
2-HEXENE, (Z)-	0.26-0.67	5.2	11
2-HEXENE, (E)-	0.27-0.66	3.1	11
3-HEXENE, (Z)-	0.27-0.66	4.3	11
3-HEXENE, (E)-	0.31-0.67	0.8	11
1-PENTENE, 2-METHYL-	0.27-0.66	3.2	16
1-PENTENE, 3-METHYL	0.24-0.65	10.5	11
1-PENTENE, 4-METHYL-	0.24-0.64	8.8	8
2-PENTENE, 2-METHYL-	0.27-0.66	4.5	11
2-PENTENE, 3-METHYL-,(Z)-	0.27-0.66	4.4	11
1-HEXENE, 4-METHYL-	0.25-0.96	44.6	47
2-PENTENE, 4-METHYL-, (Z)-	0.28-0.66	4.3	11
2-PENTENE, 4-METHYL-, (E)-	0.26-0.64	5.9	11

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
PENTANE, 3-METHYLENE-	0.28-0.97	36.5	47
1-BUTENE, 2,3-DIMETHYL-	0.23-0.65	12.6	11
1-BUTENE, 3,3-DIMETHYL-	0.33-0.64	0.7	11
2-BUTENE, 2,3-DIMETHYL-	0.38-0.64	1.3	11
1-PENTENE, 2-ETHYL-	0.30-0.98	34.4	49
1-HEPTENE	0.51-0.69	3.2	20
2-HEPTENE, (Z)-	0.26-0.67	9.2	11
2-HEPTENE, (E)-	0.30-0.67	3.0	11
3-HEPTENE, (E)-	0.25-0.68	10.4	11
1-HEXENE, 2-METHYL-	0.30-0.97	33.2	48
1-PENTENE, 3-ETHYL-	0.28-1.04	41.4	50
1-HEXENE, 3-METHYL-	0.28-0.97	39.0	47
1-HEXENE, 3-ETHYL-	0.31-0.65	10.5	14
1-HEPTENE, 4-METHYL-	0.25-0.67	10.4	11
1-BUTENE, 2,3,3-TRIMETHYL-	0.48-0.69	2.1	30
3-HEPTENE, (Z)-	0.32-0.69	2.5	11
1-OCTENE	0.33-0.67	0.7	11
2-OCTENE, (E)-	0.30-0.68	1.1	11
1-PENTENE, 2,4,4-TRIMETHYL-	0.30-0.99	37.9	47
2-PENTENE, 2,4,4-TRIMETHYL-	0.46-0.65	2.7	14
HEPTANE, 3-METHYLENE-	0.44-0.67	1.2	33
NONENE	0.37-0.98	32.7	28
1-DECENE	0.37-0.98	33.6	31
1-TRIDECENE	0.37-0.97	30.4	48
1-TETRADECENE	0.38-0.97	32.4	62
1-PENTADECENE	0.38-0.98	30.2	98
1-HEXADECENE	0.38-0.97	28.6	69
1-OCTADECENE	0.39-0.98	32.4	60
HEPTENE, 6-METHYL-	0.32-0.69	2.6	10
CYCLOPENTENE	0.27-0.80	14.4	15
CYCLOHEXENE	0.49-0.67	1.7	30
CYCLOHEPTENE	0.36-0.65	0.4	11
CYCLOOCTENE	0.34-0.66	2.0	11
2-OCTENE, (Z)	0.30-0.95	25.4	23
3-OCTENE, (E)-	0.28-0.69	7.6	11
4-OCTENE, (Z)-	0.27-0.70	10.1	10
4-OCTENE, (E)-	0.31-0.68	3.5	11
3-OCTENE, (Z)-	0.26-0.70	12.8	10
1-HEPTADECENE	0.39-0.97	28.1	66

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1-NONADECENE	0.39-0.98	32.5	76
1-EICOSENE	0.39-0.98	30.4	64
CYCLOPENTENE, 1-METHYL-	0.27-0.80	14.3	13
CYCLOPENTENE, 3-METHYL-	0.22-0.80	27.7	10
CYCLOPENTENE, 4-METHYL-	0.21-0.80	28.9	10
HEXENE, 2,3-DIMETHYL-	0.31-0.68	4.9	10
CYCLOHEXENE, 1-METHYL-4-(1-METHYLETHENYL)-, (R)-	0.31-0.80	36.6	23
CYCLOHEXENE, 1-METHYL-4-(1-METHYLETHYLIDENE)-	0.30-0.68	4.3	11
1,2-BUTADIENE	0.30-0.96	9.9	22
1,3-BUTADIENE	0.60-0.78	2.9	10
1,2-PENTADIENE	0.27-0.63	2.3	11
1,3-PENTADIENE, (Z)-	0.37-0.63	1.8	8
1,3-PENTADIENE, (E)-	0.44-0.61	0.5	8
1,4-PENTADIENE	0.26-0.62	1.2	11
2,3-PENTADIENE	0.30-0.64	3.4	11
ISOPRENE	0.56-0.63	0.6	17
1,5-HEXADIENE	0.26-0.65	2.7	11
1,2-BUTADIENE, 3-METHYL	0.33-0.63	2.0	11
1,3-CYCLOPENTADIENE, METHYL-	0.28-0.80	14.2	11
1,4-HEXADIENE	0.26-0.66	2.2	10
2,4-HEXADIENE, (E,E)-	0.43-0.65	1.1	11
1,3-CYCLOPENTADIENE	0.37-0.79	10.6	23
4,7-METHANO-1H-INDENE, 3a,4,7,7a-TETRAHYDRO-	0.32-0.67	5.4	11
1,3-CYCLOHEXADIENE, 2-METHYL-5-(1-METHYLETHYL)-	0.31-0.68	4.2	11
CYCLOHEXENE, 3-METHYLENE-6-(1-METHYLETHYL)-	0.31-0.68	4.2	11
1,3-BUTADIENE, 2,3-DIMETHYL-	0.38-0.63	1.7	21
2,4-HEXADIENE, (E,Z)-	0.33-0.65	2.0	11
1,5-HEXADIENE, 2,5-DIMETHYL-	0.35-0.68	0.9	10
2,4-HEXADIENE, 2,5-DIMETHYL-	0.48-0.80	1.6	10
1,3-CYCLOHEXADIENE	0.52-0.64	0.4	7
1,4-CYCLOHEXADIENE	0.39-0.63	1.9	10
1,5-CYCLOOCTADIENE	0.32-0.80	13.8	11
(3E)-1,3-PENTADIENE, 2-METHYL-	0.40-0.66	1.6	15
ETHYNE	0.50-0.89	2.1	5
1-PROPYNE	0.43-0.93	1.8	11
1-BUTYNE	0.44-0.85	2.6	10

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
2-BUTYNE	0.51-0.78	1.3	11
1-PENTYNE	0.35-0.78	4.2	11
3-HEXYNE	0.31-0.79	8.2	11
2-HEXYNE	0.34-0.79	6.2	11
2-PENTYNE	0.32-0.80	6.2	10
1-HEXYNE	0.27-0.80	9.2	11
1-BUTEN-3-YNE, 2-METHYL-	0.33-0.79	3.0	11
1-OCTYNE	0.34-0.82	5.6	11
1-BUTEN-3-YNE	0.38-0.80	1.5	11
1-BUTYNE, 3-METHYL-	0.40-0.79	2.0	11
1-PENTEN-3-YNE	0.29-0.79	7.8	11
1-PENTEN-4-YNE	0.30-0.80	4.0	11
BENZENE, 1,1'-(1,2-ETHYNEDIYL)BIS-	0.40-0.68	2.3	11
1-NONYNE	0.37-0.82	5.0	10
1-DECYNE	0.37-0.82	6.4	10
BENZENE	0.50-0.97	10.8	53
BENZENE, METHYL-	0.30-0.98	39.2	50
BENZENE, 1,2-DIMETHYL-	0.43-0.66	1.2	28
BENZENE, 1,3-DIMETHYL-	0.44-0.67	0.8	30
BENZENE, 1,4-DIMETHYL-	0.47-0.67	0.6	23
BENZENE, PROPYL-	0.39-0.66	2.5	49
BENZENE, 1-METHYLETHYL-	0.24-0.97	59.9	53
BENZENE, 1-ETHYL-2-METHYL-	0.30-0.97	37.2	22
BENZENE, 1-ETHYL-3-METHYL-	0.28-0.67	15.0	11
BENZENE, 1-ETHYL-4-METHYL-	0.44-0.55	0.3	21
BENZENE, 1,2,3-TRIMETHYL-	0.37-0.67	4.4	11
BENZENE, 1,2,4-TRIMETHYL-	0.35-0.68	5.5	16
BENZENE, 1,3,5-TRIMETHYL-	0.36-0.67	8.2	21
BENZENE, BUTYL-	0.38-0.64	2.8	55
BENZENE, (2-METHYLPROPYL)-	0.34-0.68	4.7	11
BENZENE, (1-METHYLPROPYL)-	0.24-0.66	51.4	29
BENZENE, (1,1-DIMETHYLETHYL)-	0.33-0.66	6.4	11
BENZENE, 1-METHYL-2-(1-METHYLETHYL)-	0.31-0.81	8.6	26
BENZENE, 1-METHYL-3-(1-METHYLETHYL)-	0.32-0.81	6.7	26
BENZENE, 1-METHYL-4-(1-METHYLETHYL)-	0.32-0.80	22.9	41
BENZENE, 1,2-DIETHYL-	0.36-0.68	5.9	11
BENZENE, 1,3-DIETHYL-	0.29-0.68	11.8	11
BENZENE, 1,4-DIETHYL-	0.35-0.68	3.1	11

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, 1,2,3,4-TETRAMETHYL-	0.39-0.69	6.9	10
BENZENE, 1,2,3,5-TETRAMETHYL-	0.37-0.69	7.8	11
BENZENE,-1,2,4,5-TETRAMETHYL-	0.52-0.68	0.8	11
BENZENE, 1-tert-BUTYL-4-ETHYL	0.34-0.71	7.2	10
BENZENE, 1,4-BIS(1,1-DIMETHYLETHYL)-	0.50-0.72	0.6	14
BENZENE, 1,3-bis(1-METHYLETHYL)-	0.31-0.69	15.2	13
BENZENE, 1,4-bis(1-METHYLETHYL)-	0.37-0.69	0.4	11
BENZENE, 1,2,4-TRIETHYL-	0.29-0.72	27.4	10
BENZENE, 1,2,3-TRIETHYL-	0.32-0.72	21.7	10
BENZENE, HEPTYL-	0.31-0.97	43.0	95
BENZENE, 1,2,3,5-TETRAETHYL	0.36-0.74	22.6	10
BENZENE, DECYL-	0.34-0.97	39.3	123
BENZENE, HEXAETHYL-	0.54-0.77	2.3	12
BENZENE, CYCLOHEXYL-	0.37-0.79	19.9	33
BIPHENYL	0.45-0.94	0.9	30
1,1':4', 1"-TERPHENYL	0.52-0.80	9.2	39
1,1':3', 1"-TERPHENYL	0.41-0.82	4.2	37
BENZENE, 1,1'-ETHYLIDENEBIS-	0.35-0.48	5.2	9
BENZENE, 1,1'-METHYLENEBIS-	0.39-0.70	1.7	20
BENZENE, (PHENYLETHYL)-	0.43-0.48	0.0	2
BENZENE, 1,1',1"-METHYLIDYNETRIS-	0.42-0.73	5.2	13
BENZENE, PENTYL-	0.30-0.98	45.7	74
BENZENE, HEXYL-	0.30-0.98	50.9	136
BENZENE, OCTYL-	0.33-0.97	35.1	52
BENZENE, NONYL-	0.34-0.98	37.7	117
BENZENE, UNDECYL-	0.34-0.97	39.2	115
BENZENE, TRIDECYL-	0.35-0.98	44.1	111
BENZENE, TETRADECYL-	0.35-0.97	34.5	58
BENZENE, DODECYL-	0.34-0.97	37.8	88
1-ETHYL-3,5-DIMETHYL BENZENE	0.29-0.69	19.3	11
2-ETHYL-1,3-DIMETHYL BENZENE	0.38-0.68	4.9	11
BENZENE, 2-ETHYL-1,4-DIMETHYL-	0.33-0.69	9.4	11
BENZENE, 1-ETHYL-,2,4-DIMETHYL-	0.32-0.69	8.7	11
4-ETHYL-1,2-DIMETHYLBENZENE	0.31-0.68	13.1	11
BENZENE, 1-ETHYL-2,3-DIMETHYL-	0.33-0.68	11.9	11
BENZENE, 1,1'-(1,1,2,2-TETRAMETHYL-1,2-ETHANEDIYL)bis-	0.49-0.80	40.9	22

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, (1-METHYLENEPROPYL)-	0.38-0.68	2.3	11
BENZENE, (1-METHYL-1-PROPENYL)-,(E)-	0.36-0.67	1.4	11
BENZENE, (1-METHYL-1-PROPENYL)-, (Z)	0.42-0.68	0.5	11
BENZENE, 1-METHYL-2-PROPYL-	0.32-0.97	30.9	55
BENZENE, 1-METHYL-3-PROPYL-	0.29-0.98	41.5	56
BENZENE, 1-METHYL-4-PROPYLBENZENE	0.32-0.98	37.6	54
BENZENE,1,1',1"-(1-ETHANYL-2-YLIDENE)tris-	0.39-0.74	11.7	10
BENZENE, 1,1',1",1'"-METHANETETRAYLTETRAKIS-	0.57-0.76	1.6	10
BENZENE, 1-ETHYL-4-(2 PHENYLETHYL)-	0.38-0.73	9.0	10
BENZENE, ETHENYL-	0.43-0.66	2.0	26
BENZENE, 1-ETHENYL-2-METHYL-	0.31-0.66	10.6	11
BENZENE, 1-ETHENYL-3-METHYL-	0.28-0.67	12.7	11
BENZENE, 1-ETHENYL-2-ETHYL-	0.30-0.69	18.6	15
BENZENE, 1-ETHENYL-3-ETHYL-	0.26-0.69	24.7	15
BENZENE, 1-ETHENYL-4-ETHYL-	0.33-0.69	4.6	15
BENZENE, 1-ETHENYL-4-METHYL-	0.36-0.66	0.5	11
BENZENE, (1-METHYLETHENYL)-	0.38-0.66	0.9	12
BENZENE, 1,3-DIETHENYL-	0.30-0.69	8.1	11
BENZENE, ETHYNYL-	0.35-0.80	8.2	12
BENZENE, 1-ETHENYL-4-(2-METHYLPROPYL)	0.34-0.71	6.0	11
BENZENE, 1-PROPENYL-,(Z)-	0.32-0.67	3.7	10
BENZENE, 1-PROPENYL-,(E)-	0.36-0.67	0.7	10
BENZENE, 1-ETHENYL-4-(1-METHYLETHENYL)-	0.33-0.71	6.6	10
NAPHTHALENE	0.47-0.85	7.0	33
NAPHTHALENE, 1-METHYL-	0.31-0.66	9.0	87
NAPHTHALENE, 2-METHYL-	0.39-0.49	1.6	31
NAPHTHALENE, 1-ETHYL-	0.35-0.80	10.1	10
NAPHTHALENE, 1,2,3,4-TETRAHYDRO-	0.38-0.62	3.2	22
NAPHTHALENE, 2,6-DIMETHYL-	0.49-0.79	9.2	22
NAPHTHALENE, 1-PHENYL-	0.38-0.80	5.6	11
NAPHTHALENE, 1-NONYL-	0.34-0.79	29.1	18

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
NAPHTHALENE, 1-BUTYL-	0.39-0.80	3.1	7
NAPHTHALENE, 1-DECYL-	0.34-0.80	11.0	8
NAPHTHALENE, 1-HEXYL-	0.34-0.80	17.9	9
NAPHTHALENE, 2,7-DIMETHYL-	0.48-0.80	21.8	22
NAPHTHALENE, 1-HEXYL-1,2,3,4-TETRAHYDRO-	0.26-0.80	30.8	11
FLUORANTHENE	0.42-0.55	1.5	12
NAPHTHALENE, 1-PROPYL-	0.35-0.80	5.7	11
NAPHTHALENE, 2-ETHYL	0.37-0.47	1.4	6
BENZENE, 1,1',1''-(1-ETHENYL-2-YLIDENE)TRIS-	0.38-0.74	20.4	21
BENZENE, 1,1',1'',1'''-(1,2-ETHENEDIYLIDENE)TETRAKIS-	0.50-0.76	13.6	21
BENZENE, 1,1'-(1,2-ETHENEDIYL)BIS-, (Z)-	0.35-0.68	10.0	10
BENZENE, 1,1'-(1,2-ETHENEDIYL)BIS-, (E)-	0.49-0.71	1.0	10
BENZENE, 1,3-DIMETHOXY-5-(2-PHENYLETHENYL)-,(E)-	0.39-0.80	9.3	15
9H-FLUORENE	0.47-0.65	2.1	16
1H-INDENE	0.40-0.80	33.5	25
ANTHRACENE	0.56-0.68	14.8	20
PHENANTHRENE	0.43-0.66	0.7	14
CHRYSENE	0.60-0.72	0.0	2
PYRENE	0.45-0.75	31.0	13
ACENAPHTHYLENE, 1,2-DIHYDRO-	0.46-0.61	4.4	14
1H-INDENE, 2,3-DIHYDRO-	0.40-0.57	4.0	18
1,3-CYCLOHEXADIENE, 1-METHYL-4-(1-METHYLETHYL)-	0.35-0.69	1.1	10
1,4-CYCLOHEXADIENE, 1-METHYL-4-(1-METHYLETHYL)-	0.34-0.68	1.2	10
BENZ(a)ANTHRACENE	0.44-0.80	8.5	19
BICYCLO(2.2.1)HEPTANE, 2,2-DIMETHYL-3-METHYLENE-	0.50-0.57	0.0	2
BICYCLO(3.1.1)HEPT-2-ENE, 2,6,6-TRIMETHYL-	0.33-0.79	20.4	19
BICYCLO(3.1.1)HEPTANE, 6,6-DIMETHYL-2-METHYLENE	0.33-0.80	23.4	11
NITROUS OXIDE	0.59-0.97	25.6	36
DINITROGEN OXIDE	0.59-0.93	26.4	24

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
HYDROGEN	0.42-0.99	21.6	52
NITROGEN	0.48-0.99	17.8	40
CARBON MONOXIDE	0.52-0.99	6.4	46
CARBON DIOXIDE	0.72-1.00	33.8	48
OXYGEN	0.35-0.98	30.6	94
SULFUR DIOXIDE	0.56-0.93	22.4	16
SULFUR TRIOXIDE	0.59-0.67	4.3	16
NITROGEN OXIDE (NO)	0.61-1.00	25.7	18
BROMINE	0.46-0.58	2.5	22
OZONE	0.30-0.62	9.6	9
PROPANAL	0.38-0.64	2.4	21
3-CYCLOHEXENE-1-CARBOXALDEHYDE	0.38-0.80	2.8	15
HEPTANAL	0.37-0.68	2.6	19
HEXANAL	0.37-0.67	0.5	11
OCTANAL	0.39-0.70	1.4	11
NONANAL	0.39-0.71	3.7	16
HEXANAL, 2-ETHYL-	0.33-0.71	2.2	11
ETHANEDIAL	0.58-0.65	0.5	12
HEXANAL, 2-METHYL-	0.39-0.70	0.8	11
HEXANAL, 3-METHYL-	0.39-0.70	0.6	11
2-PENTENAL, 2-METHYL-	0.39-0.68	2.3	10
2-HEXENAL, 2-ETHYL-	0.39-0.71	0.6	10
DECANAL	0.40-0.72	2.1	11
UNDECANAL	0.40-0.73	14.0	16
1-DODECANAL	0.40-0.73	2.8	11
TRIDECANAL	0.40-0.74	6.2	16
BUTANAL, 2-METHYL	0.50-0.58	1.3	4
3-METHYL-BUTANAL	0.41-0.67	2.7	23
2-PROPENAL	0.44-0.70	1.5	10
2-BUTENAL, (Z)-	0.29-0.80	14.1	15
trans-CROTONALDEHYDE	0.35-0.66	0.6	11
2-PROPENAL, 2-METHYL-	0.36-0.63	1.2	12
BENZENEACETALDEHYDE, alpha-METHYL-	0.42-0.69	0.4	10
BENZALDEHYDE, 2-METHYL-	0.34-0.68	5.3	11

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZALDEHYDE, 4-METHYL-	0.42-0.68	1.2	11
BENZALDEHYDE	0.36-0.64	6.9	30
BENZALDEHYDE, 2-HYDROXY-	0.43-0.69	4.9	22
BENZALDEHYDE, 4-HYDROXY-	0.48-0.48	0.0	1
1,4-BENZENEDICARBOXALDEHYDE	0.53-0.70	0.0	10
BENZALDEHYDE, 3-METHYL-	0.36-0.68	1.3	10
1,3,5-TRIOXANE, 2,4,6-TRIMETHYL-	0.49-0.69	1.9	14
2-PROPANONE	0.44-0.64	0.7	21
2-BUTANONE	0.35-1.00	12.8	67
3-PENTANONE	0.49-0.67	0.7	30
2-PENTANONE, 4-METHYL-	0.33-0.68	18.7	29
2-PENTANONE, 3-METHYL-	0.29-0.68	12.4	11
3-HEPTANONE	0.39-0.69	3.2	11
4-HEPTANONE	0.40-0.68	2.4	19
3-HEXANONE	0.37-0.67	2.2	12
2-PENTANONE	0.49-0.66	1.3	31
2-BUTANONE, 3-METHYL-	0.33-0.66	5.9	11
2-HEXANONE	0.37-0.68	2.6	16
2-HEPTANONE	0.45-0.64	1.5	18
2-HEXANONE, 5-METHYL-	0.33-0.68	8.0	12
3-PENTEN-2-ONE, 4-METHYL-	0.46-0.52	6.4	9
2-BUTANONE, 3,3-DIMETHYL-	0.39-0.66	2.5	17
4-HEPTANONE, 2,6-DIMETHYL-	0.44-0.51	4.9	7
3-PENTANONE, 2,4-DIMETHYL-	0.36-0.69	4.8	13
2-PYRROLIDINONE	0.37-0.46	2.9	23
2-PYRROLIDINONE, 1-METHYL-	0.35-0.65	23.0	24
5-NONANONE	0.42-0.72	2.6	10
2-NONANONE	0.41-0.72	3.6	12
9,10-ANTHRACENEDIONE	0.62-0.72	7.5	12
2,4-PENTANEDIONE	0.42-0.55	10.0	7
2-CYCLOHEXEN-1-ONE, 3,5,5-TRIMETHYL-	0.37-0.68	15.2	14
CYCLOPENTANONE	0.36-0.79	32.6	45
CYCLOHEXANONE	0.42-0.56	3.6	22
2-OCTANONE	0.40-0.71	2.7	10
METHANONE, DIPHENYL-	0.36-0.80	21.4	22
ETHANONE, 1-PHENYL-	0.40-0.67	6.9	40

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
2-OXETANONE	0.35-0.79	1.1	11
2(3H)-FURANONE, DIHYDRO-	0.31-0.80	36.2	22
2-OXEPANONE	0.35-0.80	21.9	16
2(3H)-FURANONE, DIHYDRO-5-METHYL-	0.33-0.80	15.2	10
2-METHYL, 3-PENTANONE-	0.36-0.68	3.0	10
3-BUTEN-2-ONE, 3-METHYL	0.39-0.65	0.2	11
(1,1'-BICYCLOHEXYL)-2-ONE	0.36-0.80	4.8	15
2,5-CYCLOHEXADIENE-1,4-DIONE	0.57-0.66	0.5	11
2-OXETANONE, 4-METHYLENE-	0.43-0.80	4.8	11
ETHENONE	0.35-0.60	0.7	10
METHANOL	0.34-0.65	6.8	35
ETHANOL	0.53-0.82	11.7	47
1-PROPANOL	0.29-0.98	82.2	57
2-PROPANOL	0.37-0.70	33.6	24
1-BUTANOL	0.33-0.97	74.6	48
1-PROPANOL, 2-METHYL-	0.39-0.99	75.6	59
2-PROPANOL, 2-METHYL-	0.58-0.89	6.7	37
1-PENTANOL	0.43-0.69	19.4	32
2-PENTANOL	0.46-0.61	10.4	25
2-BUTANOL, 2-METHYL-	0.48-0.69	5.2	39
1-PROPANOL, 2,2-DIMETHYL-	0.60-0.70	3.6	12
1-HEXANOL	0.40-0.97	54.8	41
2-HEXANOL	0.43-0.96	40.4	45
1-PENTANOL, 2-METHYL-	0.44-0.97	47.9	25
1-PENTANOL, 3-METHYL-	0.47-0.71	6.5	15
3-PENTANOL, 3-METHYL-	0.48-0.67	1.0	12
3-PENTANOL	0.40-0.97	74.3	52
1-HEXANOL, 2-ETHYL-	0.32-0.72	53.2	12
1-HEXANOL, 2-METHYL-	0.37-0.74	40.4	10
1-BUTANOL, 3-METHYL-	0.47-0.70	9.2	36
2-BUTANOL, 3-METHYL-	0.46-0.71	17.5	32
1-HEPTANOL	0.38-0.97	64.0	38
2-HEPTANOL	0.42-0.98	41.3	28
1-HEXANOL, 5-METHYL-	0.49-0.73	12.8	11
2-PENTANOL, 4-METHYL-	0.48-0.69	1.9	15
1-OCTANOL	0.40-0.97	52.4	24

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
2-OCTANOL	0.42-0.99	41.5	28
1-NONANOL	0.41-0.97	42.7	14
2-NONANOL	0.37-0.72	42.4	16
1-DECANOL	0.41-0.98	45.2	24
1-UNDECANOL	0.42-0.97	43.2	36
1-NONANOL, 8-METHYL-	0.33-0.80	50.2	10
1-DODECANOL	0.41-0.98	42.1	32
1-TRIDECANOL	0.41-0.96	34.8	51
1-TETRADECANOL	0.42-0.98	36.3	58
1-PENTADECANOL	0.42-0.98	32.7	17
1-HEXADECANOL	0.42-0.97	37.4	75
1-HEPTADECANOL	0.42-0.98	39.0	55
1-OCTADECANOL	0.42-0.98	37.5	53
1-BUTANOL, 2-ETHYL-	0.41-0.72	36.8	10
1-EICOSANOL	0.42-0.98	46.8	17
1-NONADECANOL	0.42-0.98	45.6	19
CYCLOHEXANOL	0.45-0.66	17.8	22
CYCLOHEXANOL, 1-METHYL-	0.44-0.80	40.4	22
CYCLOHEXANOL, 4-METHYL-, cis-	0.48-0.79	66.9	23
CYCLOHEXANOL, 4-METHYL-, trans-	0.47-0.79	100.2	23
CYCLOHEXANOL, 5-METHYL-2-1(1-METHYLETHYL)-[1R-{1 ALPHA, 2-BETA, 5 ALPHA}]	0.48-0.80	4.2	15
1-NAPHTHALENEMETHANOL, DECAHYDRO-5-(5-HYDROXY-3-METHYL-3-PENTENYL)-1,4a-DIMETHYL-6-METHYLENE-, [1S-[1Alpha,4aAlpha,5Alpha(E),8aBeta]]	0.40-0.66	5.2	15
Alpha,Alpha,4-TRIMETHYL-3-CYCLOHEXENE-1-METHANOL	0.37-0.68	41.2	17
CYCLOHEXANOL, 1-METHYL-4-(1-METHYLETHENYL)	0.44-0.80	43.9	16
1-NONANOL, 2-BUTYL-	0.40-0.79	39.0	15
1-UNDECANOL, 2-METHYL-	0.40-0.78	38.3	15
2-FURANMETHANOL, TETRAHYDRO-	0.46-0.46	0.0	3
2-PROPEN-1-OL	0.52-0.68	1.7	22
BENZENEMETHANOL, alpha,alpha-DIMETHYL-	0.47-0.72	6.5	15
1-OCTANOL, 2-BUTYL	0.29-0.78	61.2	15

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
PHENOL, 2,3-DIMETHYL-	0.48-0.67	14.0	11
PHENOL, 2,4-DIMETHYL	0.49-0.67	11.9	11
PHENOL, 2,5-DIMETHYL-	0.50-0.67	2.7	20
PHENOL, 2,6-DIMETHYL-	0.46-0.67	20.8	11
PHENOL, 3,4-DIMETHYL-	0.48-0.65	8.4	20
PHENOL, 3,5-DIMETHYL-	0.41-0.66	12.7	21
2-PROPYN-1-OL	0.38-0.66	24.0	13
BENZENEMETHANOL	0.40-0.48	2.9	14
PHENOL	0.42-0.99	43.4	65
PHENOL, 2-METHYL-	0.42-0.66	5.3	21
PHENOL, 3-METHYL-	0.39-0.66	3.9	39
PHENOL, 4-METHYL-	0.39-0.66	3.8	34
PHENOL, 2-ETHYL-	0.38-0.68	42.1	10
1,4-BENZENEDIOL	0.54-0.80	3.6	15
PHENOL, 4-ETHYL-	0.44-0.68	37.0	11
PHENOL, 4-(1,1-DIMETHYLETHYL)-	0.51-0.70	18.6	10
PHENOL, 4,4'-(1-METHYLETHYLIDENE)bis-	0.51-0.98	59.2	52
PHENOL, NONYL-	0.35-0.61	76.9	26
1,2-ETHANEDIOL	0.36-0.63	19.5	80
ETHANOL, 2,2'-OXYBIS-	0.39-0.57	5.7	21
ETHANOL, 2,2'-(1,2-ETHANEDIYLBIS(OXY))BIS-	0.29-0.87	43.2	63
ETHANOL, 2,2'-(OXYBIS(2,1-ETHANEDIYLOXY))BIS-	0.37-0.54	2.3	12
1,2-PROPANEDIOL	0.37-0.74	62.6	33
1,3-PROPANEDIOL	0.34-0.67	38.3	15
PROPANOL, OXYBIS-	0.36-0.80	67.1	17
1,3-PROPANEDIOL, 2,2-DIMETHYL-	0.64-0.80	2.8	15
PROPANOL,((1-METHYL-1,2-ETHANEDIYL)bis(oxy))bis-	0.40-0.80	35.6	6
1,3-PROPANEDIOL, 2-METHYL-	0.43-0.69	4.4	3
1,2-BUTANEDIOL	0.43-0.64	22.3	10
2,4-PENTANEDIOL, 2-METHYL-	0.35-0.76	71.2	15
1,2,3-PROPANETRIOL	0.27-0.56	93.3	83
1,2,4-BUTANETRIOL	0.43-0.43	0.0	1
1,2-BENZENEDIOL, 4-(1,1-DIMETHYLETHYL-)	0.43-0.80	13.1	15

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1,3-PENTANEDIOL, 2,2,4-TRIMETHYL	0.48-0.48	0.0	1
1,3-PENTANEDIOL, 2-METHYL	0.38-0.76	39.9	15
2,3-BUTANEDIOL	0.46-0.74	35.4	11
2-BUTENE-1,4-DIOL, (Z)-	0.42-0.74	42.7	25
1,4-BUTANEDIOL	0.44-0.70	12.9	14
1,5-PENTANEDIOL	0.36-0.64	59.6	47
1,6-HEXANEDIOL	0.40-0.63	59.2	37
1,2-BENZENEDIOL	0.50-0.66	1.2	14
1,3-BENZENEDIOL	0.51-0.66	3.6	9
1,3-PROPANEDIOL, 2,2-BIS(HYDROXYMETHYL)-	0.33-0.81	35.0	17
1,3-PROPANEDIOL, 2-ETHYL-2-(HYDROXYMETHYL)-	0.49-0.49	0.0	1
1,2,3-BENZENETRIOL	0.49-0.70	17.0	10
FORMIC ACID	0.48-0.64	1.8	20
ACETIC ACID	0.49-0.68	7.8	51
PROPANOIC ACID	0.46-0.69	1.2	43
DECANOIC ACID	0.42-0.74	12.4	14
BUTANOIC ACID	0.45-0.70	3.9	40
BUTANOIC ACID, 2-METHYL-, (+ -)	0.46-0.70	2.8	12
PENTANOIC ACID	0.45-0.57	2.9	23
NONANOIC ACID	0.41-0.51	1.3	10
PROPANOIC ACID, 2-METHYL-	0.45-0.70	1.3	34
BUTANOIC ACID, 3-METHYL-	0.39-0.72	13.4	16
HEXANOIC ACID	0.44-0.56	1.1	31
HEXANOIC ACID, 2-METHYL-	0.66-0.80	2.2	15
1,4-CYCLOHEXANEDICARBOXYLIC ACID, trans-	0.42-0.52	4.3	10
OCTANOIC ACID	0.41-0.76	18.5	12
UNDECANOIC ACID	0.41-0.71	7.6	10
CYCLOPENTANEACETIC ACID	0.58-0.74	2.5	10
PROPANOIC ACID, 2,2'-OXYBIS-	0.44-0.62	5.4	16
DODECANOIC ACID	0.42-0.78	16.7	11
TRIDECANOIC ACID	0.44-0.48	1.9	8
TETRADECANOIC ACID	0.44-0.60	4.8	19
2-BUTENOIC ACID, (Z)-	0.45-0.68	1.5	11
2-BUTENOIC ACID, (E)-	0.52-0.68	0.7	11
OCTADECANOIC ACID	0.43-0.59	6.8	18
2-PROPENOIC ACID	0.42-0.75	6.5	24
2-PROPENOIC ACID, 2-METHYL-	0.42-0.65	0.5	11

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
9-OCTADECENOIC ACID(Z)-	0.38-0.60	9.9	26
9,12-OCTADECADIENOIC ACID(Z,Z)-	0.35-0.80	50.7	21
BENZOIC ACID	0.53-0.56	7.7	7
BENZOIC ACID, 2-METHYL-	0.55-0.63	1.4	7
BENZOIC ACID, 4-METHYL-	0.59-0.70	1.3	11
BENZOIC ACID, 2-HYDROXY-	0.58-0.80	2.6	16
HEXANEDIOIC ACID	0.54-0.58	0.0	2
2-BUTENEDIOIC ACID (Z)-	0.52-0.73	2.6	11
1,2-BENZENEDICARBOXYLIC ACID	0.58-0.74	3.7	11
ETHANEPEROXOIC ACID	0.53-0.68	2.1	5
ACETIC ACID, ANHYDRIDE	0.45-0.67	0.6	30
PROPANOIC ACID, ANHYDRIDE	0.44-0.70	0.8	26
BUTANOIC ACID, ANHYDRIDE	0.46-0.64	1.2	15
2,5-FURANDIONE, DIHYDRO-	0.49-0.66	0.2	11
2H-PYRAN-2,6(3H)-DIONE, DIHYDRO-	0.39-0.63	19.6	14
1,3-ISOBENZOFURANDIONE	0.51-0.70	24.9	21
2,5-FURANDIONE	0.46-0.59	2.3	8
5-ISOBENZOFURANCARBOXYLIC ACID, 1,3-DIHYDRO-1,3-DIOXO-	0.49-0.74	30.9	16
FORMIC ACID, METHYL ESTER	0.56-0.62	1.9	17
FORMIC ACID, ETHYL ESTER	0.54-0.61	0.6	15
FORMIC ACID, PROPYL ESTER	0.51-0.66	1.4	25
FORMIC ACID, BUTYL ESTER	0.52-0.66	2.9	9
FORMIC ACID, 2-METHYLPROPYL ESTER	0.53-0.67	0.7	11
FORMIC ACID, PENTYL ESTER	0.35-0.69	5.4	13
FORMIC ACID, OCTYL ESTER	0.36-0.72	8.9	13
FORMIC ACID, NONYL ESTER	0.37-0.74	8.2	10
FORMIC ACID, DECYL ESTER	0.37-0.75	8.6	10
FORMIC ACID, ETHENYL ESTER	0.40-0.64	0.7	11
ACETIC ACID, METHYL ESTER	0.54-0.82	4.4	38
ACETIC ACID, ETHYL ESTER	0.52-0.90	6.9	28
ACETIC ACID, PROPYL ESTER	0.50-0.86	8.5	23
ACETIC ACID, BUTYL ESTER	0.50-0.63	2.3	35
ACETIC ACID, 2-METHYLPROPYL ESTER	0.52-0.66	2.6	9
1-BUTANOL, 3-METHYL-, ACETATE	0.48-0.79	2.7	20
ACETIC ACID, 2-PROPENYL ESTER	0.53-0.83	15.3	25
ACETIC ACID, 1-METHYLETHYL ESTER	0.38-0.68	4.3	16

Table A2. Liquid viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
ACETIC ACID, 1-METHYLPROPYL ESTER	0.40-0.69	1.8	11
ACETIC ACID, ETHENYL ESTER	0.53-0.64	0.4	13
PROPANOIC ACID, METHYL ESTER	0.52-0.66	1.1	20
PROPANOIC ACID, ETHYL ESTER	0.50-0.67	0.9	27
PROPANOIC ACID, PROPYL ESTER	0.35-0.68	4.6	16
PROPANOIC ACID, BUTYL ESTER	0.31-0.70	13.4	13
BUTANOIC ACID, PROPYL ESTER	0.46-0.93	16.8	25
PROPANOIC ACID, ETHENYL ESTER	0.42-0.66	0.2	11
BUTANOIC ACID, METHYL ESTER	0.49-0.67	1.7	36
BUTANOIC ACID, ETHYL ESTER	0.48-0.69	0.8	28
PROPANOIC ACID, 2-METHYL-, PROPYL ESTER	0.36-0.71	5.9	12
2-PROPENOIC ACID, METHYL ESTER	0.51-0.69	6.6	16
ACRYLIC ACID, ETHYL ESTER	0.50-0.71	1.7	9
2-PROPENOIC ACID, PROPYL ESTER	0.48-0.67	0.3	11
NONANOIC ACID, BUTYL ESTER	0.35-0.77	16.7	10
PENTANOIC ACID, BUTYL ESTER	0.29-0.72	26.7	20
BUTANOIC ACID, 3-METHYL-, ETHYL ESTER	0.30-0.69	16.0	11
2-PROPENOIC ACID, 2-METHYL-, METHYL ESTER	0.49-0.69	3.0	11
METHACRYLIC ACID, ETHYL ESTER	0.39-0.66	4.2	21
2-PROPENOIC ACID, 2-METHYL-, PROPYL ESTER	0.31-0.69	9.7	10
1,2-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.29-0.46	44.4	41
1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER	0.34-0.37	0.0	2
ACETIC ACID, PENTYL ESTER	0.34-0.80	22.8	39
ACETIC ACID, 2-ETHYLHEXYL ESTER	0.28-0.73	28.8	12
ACETIC ACID, PHENYLMETHYL ESTER	0.32-0.70	23.6	13

Table A.3. Influence of variation in temperature range used to regress the SVRC model parameters

	Reduced Temperature Range Used	α
Base Case		
2-Methylhexane	0.52-0.69	-0.0813
Dodecane	0.40-0.65	-0.4378
Tridecane	0.40-0.70	-0.4609
Tetradecane	0.40-0.61	-0.3977
Case-I		
2-Methylhexane	0.52-0.67	-0.0967
Dodecane	0.42-0.54	-0.3718
Tridecane	0.41-0.55	-0.4269
Tetradecane	0.40-0.54	-0.3593
Case-II		
2-Methylhexane	0.53-0.67	0.0009
Dodecane	0.43-0.54	-0.3628
Tridecane	0.43-0.55	-0.3027
Tetradecane	0.40-0.54	-0.3646
Case-III		
2-Methylhexane	0.53-0.65	0.0105
Dodecane	0.43-0.48	-0.0175
Tridecane	0.43-0.49	-0.0769
Tetradecane	0.40-0.54	-0.3624

Table A.4. Sensitivity of liquid viscosity predictions to errors in model parameters

Error introduced in the model parameter (α) (Deviation from regressed values)	**-75%**	**-50%**	**-25%**	**-5%**	**0%**	**5%**	**25%**	**50%**	**75%**
Overall %AAD in predictions	9.4	6	2.9	0.9	0.7	0.9	2.8	5.2	7.4

Table A.5. Comparison of liquid viscosity predictions for selected compounds

Compound name	**Reduced Temperature Range**	**VCL Method (%AAD)*⁺**	**SVRC-QSPR Model (%AAD)**
Dodecane	0.40-0.65	2.1	1.7
Tridecane	0.40-0.70	3.0	1.1
Tetradecane	0.40-0.61	4.3	1.6
Hexadecane	0.41-0.78	16.4	0.9
Heptadecane	0.40-0.78	13.5	2.7

*Method recommended by Reid, Sherwood and Prausnitz (Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Gases and Liquids. 4 ed. 1987: McGraw Hill.)

+ VCL – Van Velzen, Cardozo, and Langenkamp

APPENDIX B

THE SVRC-QSPR MODEL FOR VAPOR VISCOSITIES: DATABASE USED FOR MODEL DEVELOPMENT AND VALIDATION

Table B1. Vapor viscosity data used for model development

Compound Name	Reduced Temperature Range	Data points	Classification
PENTANE	0.64-1.00	9	TR
HEPTANE, 2-METHYL-	0.64-0.98	7	TR
HEPTANE, 3-METHYL-	0.63-0.97	6	PR
HEPTANE, 4-METHYL-	0.64-0.94	6	TR
NONANE	0.46-0.96	16	TR
TRIDECANE	0.41-1.00	17	PR
TETRADECANE	0.39-0.97	22	TR
PENTADECANE	0.42-0.99	17	TR
HEXADECANE	0.38-0.97	20	TR
CYCLOPROPANE	0.74-1.00	21	TR
CYCLOPENTANE	0.58-0.89	13	PR
CYCLOHEXANE	0.58-1.00	13	TR
ETHENE	0.68-0.97	8	PR
1-PROPENE	0.53-0.97	21	TR
BENZENE	0.51-0.98	49	TR
BENZENE, METHYL-	0.56-0.89	15	TR
SULFUR DIOXIDE	0.58-0.98	12	TR
2-PROPANOL	0.77-0.97	9	TR
ETHANE, CHLORO-	0.46-0.92	11	PR
METHANE, CHLOROTRIFLUORO	0.81-0.99	6	TR
METHANE, BROMO-	0.59-0.84	11	TR
CARBON DISULFIDE	0.50-0.98	11	TR
WATER-d2	0.43-0.58	11	TR
ETHANE, 1,1-DIFLUORO (R-152A)	0.63-0.97	35	PR
ETHANE, 1,1,1,2-TETRAFLUORO	0.65-0.92	14	TR
ETHANE, DIFLUORO	0.64-0.98	13	PR
ETHANE, PENTAFLUORO	0.66-0.98	13	TR
ETHANE, 1-CHLORO-1,2,2,2-TETRAFLUORO	0.68-0.83	14	TR

Table B2. Vapor viscosity data used for external validation

Compound Name	Reduced Temperature Range	%AAD	Data points
METHANE	0.47-1.00	4.2	24
ETHANE	0.60-0.99	1.5	48
PROPANE	0.23-0.98	3.4	60
PROPANE, 2-METHYL-	0.28-0.98	3.7	57
BUTANE	0.32-0.99	6.1	65
PENTANE	0.64-1.00	1.6	24
BUTANE, 2-METHYL-	0.25-1.00	2.8	41
PROPANE, 2,2-DIMETHYL-	0.58-1.00	2.8	36
HEXANE	0.64-0.99	1.0	15
PENTANE, 2-METHYL-	0.55-0.94	2.0	7
PENTANE, 3-METHYL-	0.67-0.93	0.4	3
BUTANE, 2,2-DIMETHYL-	0.66-0.93	2.1	8
BUTANE, 2,3-DIMETHYL-	0.60-0.93	1.1	9
HEPTANE	0.63-0.98	2.1	17
HEXANE, 2-METHYL-	0.53-0.96	1.6	8
HEXANE, 3-METHYL-	0.68-0.92	0.2	3
PENTANE, 3-ETHYL-	0.68-0.91	0.3	3
PENTANE, 2,2-DIMETHYL-	0.68-0.92	0.3	3
PENTANE, 2,3-DIMETHYL-	0.68-0.91	0.0	3
PENTANE, 2,4-DIMETHYL-	0.66-0.93	0.5	10
PENTANE, 3,3-DIMETHYL-	0.67-0.91	0.2	3
BUTANE, 2,2,3-TRIMETHYL-	0.65-0.85	0.8	4
OCTANE	0.61-0.99	4.5	20
HEPTANE, 2-METHYL-	0.64-0.98	1.6	10
HEPTANE, 3-METHYL-	0.63-0.97	1.5	9
HEPTANE, 4-METHYL-	0.64-0.94	2.4	9
HEXANE, 3-ETHYL-	0.69-0.91	0.2	3
HEXANE, 2,2-DIMETHYL-	0.69-0.92	0.2	3
HEXANE, 2,3-DIMETHYL-	0.69-0.91	0.2	3
HEXANE, 2,4-DIMETHYL-	0.69-0.91	0.1	3
HEXANE, 2,5-DIMETHYL-	0.70-0.92	0.1	3
HEXANE, 3,3-DIMETHYL-	0.69-0.90	0.2	3
HEXANE, 3,4-DIMETHYL-	0.69-0.90	0.1	3
PENTANE, 3-ETHYL-2-METHYL-	0.69-0.90	0.2	3
PENTANE, 3-ETHYL-3-METHYL-	0.32-0.88	4.7	5
PENTANE, 2,2,3,TRIMETHYL-	0.68-0.90	0.1	3
PENTANE, 2,2,4-TRIMETHYL-	0.51-0.91	4.0	18
PENTANE, 2,3,3-TRIMETHYL-	0.68-1.00	0.4	4
PENTANE, 2,3,4-TRIMETHYL-	0.68-0.90	0.1	3
BUTANE, 2,2,3,3-TETRAMETHYL-	0.66-0.99	0.6	7
NONANE	0.46-0.96	1.8	17

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
HEXANE, 2,2,5-TRIMETHYL-	0.29-0.94	6.7	5
HEPTANE, 3,3,5-TRIMETHYL-	0.27-0.88	6.3	5
HEXANE,2,4,4-TRIMETHYL-	0.28-1.00	7.9	11
PENTANE, 3,3-DIETHYL-	0.69-0.97	0.3	4
PENTANE, 2,2,3,3,-TETRAMETHYL-	0.43-0.97	3.1	5
PENTANE, 2,2,3,4-TETRAMETHYL-	0.26-0.89	7.1	5
PENTANE, 2,2,4,4-TETRAMETHYL-	0.36-0.97	4.7	5
PENTANE, 2,3,3,4-TETRAMETHYL-	0.28-0.89	7.0	10
TETRACOSANE, 2,6,10,15,19,23-HEXAMETHYL-	0.27-0.98	3.3	9
DECANE	0.45-0.99	1.9	19
HEXANE, 2,2,3,3-TETRAMETHYL-	0.35-0.91	4.0	5
HEXANE, 2,2,5,5-TETRAMETHYL-	0.45-0.87	1.7	4
UNDECANE	0.50-0.94	2.2	10
DODECANE	0.47-0.99	3.1	12
TRIDECANE	0.41-1.00	0.5	17
TETRADECANE	0.39-0.97	0.9	22
PENTADECANE	0.39-0.99	0.6	18
HEXADECANE	0.38-0.97	2.0	26
HEPTADECANE	0.54-0.95	7.1	10
OCTADECANE	0.54-0.95	8.0	10
NONADECANE	0.53-0.95	16.6	13
OCTANE, 2,2-DIMETHYL-	0.37-0.89	3.7	5
EICOSANE	0.52-0.95	13.7	10
HENEICOSANE	0.40-0.99	1.8	9
DOCOSANE	0.40-0.98	1.8	9
TRICOSANE	0.40-0.97	8.4	9
TETRACOSANE	0.40-1.00	7.3	18
PENTACOSANE	0.40-0.99	10.3	10
HEXACOSANE	0.40-0.98	10.5	10
HEPTACOSANE	0.48-0.97	0.8	3
OCTACOSANE	0.40-0.96	8.0	18
NONACOSANE	0.48-0.96	0.9	3
NONANE, 3-METHYL-	0.31-0.97	7.1	6
NONANE, 2-METHYL-	0.33-0.98	6.7	6
NONANE, 4-METHYL-	0.29-0.96	7.9	6
NONANE, 5-METHYL	0.30-0.97	7.3	6
NONANE, 2,2,4,4,6,8,8-HEPTAMETHYL-	0.24-0.91	2.7	6
OCTANE, 2-METHYL-	0.33-0.95	5.5	5
OCTANE, 3-METHYL-	0.71-0.90	0.8	3

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
OCTANE, 4-METHYL-	0.71-0.91	0.4	3
3-ETHYLHEPTANE	0.27-0.98	7.1	6
HEPTANE, 2,2-DIMETHYL-	0.28-0.93	7.0	5
UNDECANE, 3-METHYL-	0.33-0.99	6.6	6
CYCLOPROPANE	0.69-1.00	0.8	29
CYCLOBUTANE	0.62-0.93	2.1	7
CYCLOPENTANE	0.35-0.89	2.8	17
CYCLOPENTANE, METHYL-	0.65-0.89	0.2	3
CYCLOPENTANE, ETHYL-	0.66-0.99	0.1	4
CYCLOPENTANE, 1,1-DIMETHYL-	0.37-0.95	0.8	5
CYCLOPENTANE, 1,2-DIMETHYL-, cis-	0.66-0.99	0.1	4
CYCLOPENTANE, 1,2-DIMETHYL-, trans-	0.66-0.89	0.1	3
CYCLOPENTANE, 1,3-DIMETHYL-, cis-	0.25-0.88	1.2	5
CYCLOPENTANE, 1,3-DIMETHYL-, trans-	0.25-0.87	1.1	5
CYCLOPENTANE, PROPYL-	0.26-0.99	1.3	6
CYCLOPENTANE,(1-METHYLETHYL)-	0.27-0.90	1.3	5
CYCLOPENTANE, 1-ETHYL-1-METHYL-	0.22-0.97	1.8	6
CYCLOPENTANE, 1-BUTYL-	0.27-0.95	1.8	11
CYCLOHEXANE	0.58-1.00	0.4	13
CYCLOHEXANE, METHYL-	0.65-0.98	0.1	4
CYCLOHEXANE, ETHYL-	0.27-0.88	1.9	5
CYCLOHEXANE, 1,1-DIMETHYL-	0.66-0.97	0.1	4
CYCLOHEXANE, 1,2-DIMETHYL-, cis-	0.67-0.96	0.0	4
CYCLOHEXANE, 1,2-DIMETHYL-, trans-	0.67-0.97	0.2	4
CYCLOHEXANE, 1,3-DIMETHYL-, cis-	0.67-0.97	0.2	4
CYCLOHEXANE, 1,3-DIMETHYL-, trans-	0.67-0.97	0.1	4
CYCLOHEXANE, 1,4-DIMETHYL-, cis-	0.66-0.97	0.2	4
CYCLOHEXANE, 1,4-DIMETHYL-, trans-	0.40-0.98	0.5	5
CYCLOHEXANE, 1,3,5-TRIMETHYL-, trans	0.31-0.91	0.6	5
CYCLOHEXANE, PROPYL-	0.67-0.94	2.1	5
CYCLOHEXANE, (1-METHYL ETHYL)-	0.29-0.94	1.3	6
CYCLOHEXANE,-1,2,3,4-TETRAMETHYL-	0.31-0.87	0.8	5
CYCLOHEXANE, BUTYL-	0.30-0.97	5.7	8

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
cis-DECALIN	0.33-0.94	0.7	6
trans-DECALIN	0.35-0.97	0.5	6
1,1'-BICYCLOHEXYL	0.71-0.97	0.2	5
CYCLOHEXANE, 1,1-DIETHYL-	0.27-0.98	2.2	7
CYCLOHEXANE, DECYL-	0.36-0.94	1.4	7
CYCLOHEPTANE	0.44-0.98	0.7	5
CYCLOOCTANE	0.45-0.93	0.3	10
CYCLOHEXANE, trans-1,4-DIETHYL	0.31-0.93	1.0	8
HEPTANE, 2,6-DIMETHYL-	0.29-0.86	5.7	5
3-ETHYLPENTANE, 2-2-DIMETHYL-	0.29-0.99	7.3	6
3-ETHYLPENTANE, 2,4-DIMETHYL-	0.26-0.97	8.6	6
ETHENE	0.60-0.99	0.8	41
1-PROPENE	0.52-1.00	1.6	58
1-TRIACONTENE	0.39-0.95	0.9	11
1-BUTENE	0.70-0.94	0.2	6
2-BUTENE, (Z)-	0.67-0.90	0.5	10
2-BUTENE, (E)-	0.68-0.99	1.9	14
1-PROPENE, 2-METHYL-	0.32-0.96	1.7	28
1-PENTENE	0.23-0.99	2.1	26
2-PENTENE, (Z)-	0.35-0.88	1.0	4
2-PENTENE, (E)-	0.28-0.82	1.3	4
1-BUTENE, 2-METHYL-	0.29-0.91	3.4	4
1-BUTENE, 3-METHYL-	0.60-0.96	1.3	28
2-BUTENE, 2-METHYL-	0.30-0.91	2.2	17
1-HEXENE	0.50-0.99	3.6	28
2-HEXENE, (Z)-	0.67-0.92	0.2	3
2-HEXENE, (E)-	0.67-0.92	0.2	3
3-HEXENE, (Z)-	0.27-0.94	7.5	5
3-HEXENE, (E)-	0.31-0.97	4.6	5
1-PENTENE, 2-METHYL-	0.27-0.84	0.6	4
1-PENTENE, 3-METHYL	0.24-0.95	0.7	5
1-PENTENE, 4-METHYL-	0.66-0.93	0.1	3
2-PENTENE, 2-METHYL-	0.66-0.92	0.2	3
2-PENTENE, 3-METHYL-,(Z)-	0.27-0.94	1.6	5
1-HEXENE, 4-METHYL-	0.25-0.89	2.2	5
2-PENTENE, 4-METHYL-, (Z)-	0.66-0.93	0.3	3
2-PENTENE, 4-METHYL-, (E)-	0.66-0.93	0.1	3
PENTANE, 3-METHYLENE-	0.28-0.84	1.8	4

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1-BUTENE, 2,3-DIMETHYL-	0.23-0.82	3.4	4
1-BUTENE, 3,3-DIMETHYL-	0.33-0.85	1.6	4
2-BUTENE, 2,3-DIMETHYL-	0.38-0.88	2.9	4
1-PENTENE, 2-ETHYL-	0.31-0.92	1.4	5
1-HEPTENE	0.47-0.98	3.2	30
2-HEPTENE, (Z)-	0.68-0.90	0.1	3
2-HEPTENE, (E)-	0.30-0.91	6.0	5
3-HEPTENE, (E)-	0.25-0.89	7.4	5
1-HEXENE, 2-METHYL-	0.32-0.93	5.7	5
1-PENTENE, 3-ETHYL-	0.28-0.92	1.1	5
1-HEXENE, 3-METHYL-	0.28-0.92	2.1	5
1-HEXENE, 3-ETHYL-	0.32-0.95	0.2	9
1-HEPTENE, 4-METHYL-	0.30-0.93	2.9	9
1-BUTENE, 2,3,3-TRIMETHYL-	0.31-0.93	1.7	5
3-HEPTENE, (Z)-	0.68-0.91	0.1	3
1-OCTENE	0.50-0.95	2.2	27
2-OCTENE, (E)-	0.69-0.90	0.0	3
1-PENTENE, 2,4,4-TRIMETHYL-	0.33-0.99	6.0	5
2-PENTENE, 2,4,4-TRIMETHYL-	0.30-0.97	2.1	5
HEPTANE, 3-METHYLENE-	0.33-0.97	0.9	5
NONENE	0.32-0.98	7.0	24
1-DECENE	0.34-0.91	3.2	5
1-UNDECENE	0.35-0.96	2.6	6
1-DODECENE	0.36-0.94	1.6	6
1-TRIDECENE	0.37-0.92	1.2	6
1-TETRADECENE	0.38-0.90	1.1	6
1-PENTADECENE	0.38-1.00	1.5	7
1-HEXADECENE	0.38-0.98	1.4	7
1-OCTADECENE	0.39-0.95	1.2	7
HEPTENE, 6-METHYL-	0.32-0.98	0.2	5
CYCLOPENTENE	0.27-0.84	0.1	4
CYCLOHEXENE	0.64-0.98	0.3	4
trans-2-EICOSENE	0.38-1.00	0.8	10
trans-2-PENTADECENE	0.77-0.95	0.3	4
CYCLOHEPTENE	0.36-0.95	1.0	5
CYCLOOCTENE	0.34-0.89	0.6	5
2-OCTENE, (Z)	0.30-0.95	6.5	5

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
3-OCTENE, (E)-	0.69-0.90	0.1	3
4-OCTENE, (Z)-	0.27-0.93	7.4	5
4-OCTENE, (E)-	0.31-0.89	5.2	5
3-OCTENE, (Z)-	0.26-0.93	7.9	5
1-HEPTADECENE	0.39-0.93	1.1	6
1-NONADECENE	0.39-0.94	1.2	7
1-EICOSENE	0.39-0.93	1.1	7
CYCLOHEXENE, 4-ETHENYL-	0.67-0.97	0.1	4
CYCLOPENTENE, 1-METHYL-	0.27-0.97	1.0	5
CYCLOPENTENE, 3-METHYL-	0.22-0.97	4.2	5
CYCLOPENTENE, 4-METHYL-	0.21-0.96	2.8	5
HEXENE, 2,3-DIMETHYL-	0.31-0.96	1.6	5
CYCLOHEXENE, 1-METHYL-4-(1-METHYLETHENYL)-, (R)-	0.31-0.92	2.3	6
CYCLOHEXENE, 1-METHYL-4-(1-METHYLETHYLIDENE)-	0.30-0.90	1.1	6
CYCLOHEXENE,1-(2-PROPENYL)	0.31-0.87	1.9	5
1,2-BUTADIENE	0.30-0.91	1.7	10
1,3-BUTADIENE	0.39-0.97	0.6	8
1,2-PENTADIENE	0.27-0.96	5.5	5
1,3-PENTADIENE, (Z)-	0.64-0.91	0.2	3
1,3-PENTADIENE, (E)-	0.63-0.90	0.1	3
1,4-PENTADIENE	0.62-0.92	0.4	3
2,3-PENTADIENE	0.30-0.98	1.9	5
ISOPRENE	0.64-0.92	0.1	3
1,5-HEXADIENE	0.26-0.94	3.9	5
1,2-BUTADIENE, 3-METHYL	0.33-0.84	1.6	4
1,3-CYCLOPENTADIENE, METHYL-	0.28-0.91	1.3	5
1,4-HEXADIENE	0.26-0.83	1.3	4
2,4-HEXADIENE, (E,E)-	0.43-0.86	0.3	4
1,3-CYCLOPENTADIENE	0.37-0.99	4.1	9
4,7-METHANO-1H-INDENE, 3a,4,7,7a-TETRAHYDRO-	0.46-0.99	0.5	6
1,3-CYCLOHEXADIENE, 2-METHYL-5-(1-METHYLETHYL)-	0.34-0.94	0.8	6
CYCLOHEXENE, 3-METHYLENE-6-(1-METHYLETHYL)-	0.34-0.94	1.0	6
1,3-BUTADIENE, 2,3-DIMETHYL-	0.38-0.98	0.7	11
2,4-HEXADIENE, (E,Z)-	0.33-0.94	0.6	5
3-METHYL-1,4-PENTADIENE	0.27-0.89	0.2	6

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1,5,9-CYCLODODECATRIENE,(E,E,Z)	0.34-0.90	0.2	6
1,5-HEXADIENE, 2,5-DIMETHYL-	0.35-0.98	5.2	5
2,4-HEXADIENE, 2,5-DIMETHYL-	0.48-0.88	1.3	4
1,3-CYCLOHEXADIENE	0.29-0.88	3.9	5
1,4-CYCLOHEXADIENE	0.39-1.00	0.5	5
1,5-CYCLOOCTADIENE	0.32-0.93	1.3	6
(3E)-1,3-HEXADIENE	0.40-0.94	0.4	6
(3E)-1,3-PENTADIENE, 2-METHYL-	0.40-0.93	2.2	6
ETHYNE	0.63-0.98	1.5	10
1-PROPYNE	0.43-0.93	1.5	16
1-BUTYNE	0.48-0.85	0.1	9
2-BUTYNE	0.37-0.98	4.6	10
1-PENTYNE	0.35-0.87	1.1	4
3-HEXYNE	0.31-0.92	1.2	5
2-HEXYNE	0.34-0.93	5.2	5
2-PENTYNE	0.32-0.96	0.8	5
1-HEXYNE	0.27-0.93	6.6	5
1-BUTEN-3-YNE, 2-METHYL-	0.33-0.83	2.3	4
1-OCTYNE	0.34-0.96	5.3	5
1-BUTEN-3-YNE	0.38-0.92	2.3	4
1-BUTYNE, 3-METHYL-	0.40-0.92	1.6	4
1-PENTEN-3-YNE	0.29-0.94	4.2	5
1-PENTEN-4-YNE	0.30-0.97	1.9	5
BENZENE, 1,1'-(1,2-ETHYNEDIYL)BIS-	0.69-0.99	0.2	7
1-NONYNE	0.37-0.97	1.8	25
1-DECYNE	0.37-0.97	2.0	24
BENZENE	0.49-0.98	0.7	50
BENZENE, METHYL-	0.30-0.92	3.7	20
BENZENE, ETHYL-	0.29-0.93	3.2	12
BENZENE, 1,2-DIMETHYL-	0.39-0.92	3.0	8
BENZENE, 1,3-DIMETHYL-	0.37-0.92	3.8	8
BENZENE, 1,4-DIMETHYL-	0.44-0.98	5.0	13
BENZENE, PROPYL-	0.27-0.99	4.9	12
BENZENE, 1-METHYLETHYL-	0.28-0.99	7.2	21
BENZENE, 1-ETHYL-2-METHYL-	0.30-0.99	3.6	6
BENZENE, 1-ETHYL-3-METHYL-	0.28-1.00	4.2	6

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, 1-ETHYL-4-METHYL-	0.33-0.88	1.4	5
BENZENE, 1,2,3-TRIMETHYL-	0.37-0.88	0.7	5
BENZENE, 1,2,4-TRIMETHYL-	0.35-0.88	0.5	5
BENZENE, 1,3,5-TRIMETHYL-	0.36-0.90	2.0	18
BENZENE, BUTYL-	0.28-0.97	2.5	6
BENZENE, (2-METHYLPROPYL)-	0.34-0.87	0.3	5
BENZENE, (1-METHYLPROPYL)-	0.67-0.92	0.3	4
BENZENE, (1,1-DIMETHYLETHYL)-	0.67-0.92	0.1	4
BENZENE, 1-METHYL-2-(1-METHYLETHYL)-	0.31-0.98	3.5	13
BENZENE, 1-METHYL-3-(1-METHYLETHYL)-	0.32-1.00	3.0	14
BENZENE, 1-METHYL-4-(1-METHYLETHYL)-	0.32-0.99	3.1	14
BENZENE, 1,2-DIETHYL-	0.68-0.93	0.2	4
BENZENE, 1,3-DIETHYL-	0.69-0.93	0.1	4
BENZENE, 1,4-DIETHYL-	0.35-0.87	0.9	5
BENZENE, 1,2,3,4-TETRAMETHYL-	0.39-0.97	0.7	6
BENZENE, 1,2,3,5-TETRAMETHYL-	0.37-0.92	0.9	6
BENZENE,-1,2,4,5-TETRAMETHYL-	0.52-0.95	0.1	5
BENZENE, 1-tert-BUTYL-4-ETHYL	0.34-0.97	1.3	6
BENZENE, 1,4-BIS(1,1-DIMETHYLETHYL)-	0.50-0.90	0.5	5
BENZENE, PENTAMETHYL-	0.45-0.97	0.6	6
BENZENE, 1,3-bis(1-METHYLETHYL)-	0.70-0.92	0.1	4
BENZENE, 1,4-bis(1-METHYLETHYL)-	0.70-1.00	0.1	5
BENZENE, 1,2,4-TRIETHYL-	0.29-0.94	2.0	6
BENZENE, HEXAMETHYL-	0.58-0.99	0.1	6
BENZENE, 1,2,3-TRIETHYL-	0.32-0.95	2.3	6
BENZENE, HEPTYL-	0.32-0.96	2.1	7
BENZENE, 1,2,3,5-TETRAETHYL	0.36-0.94	1.2	6
BENZENE, DECYL-	0.34-1.00	1.8	7
BENZENE, PENTAETHYL	0.28-0.89	0.8	6
BENZENE, HEXAETHYL-	0.54-0.99	0.1	6
BENZENE, CYCLOHEXYL-	0.38-0.91	1.1	6
BIPHENYL	0.44-0.94	10.3	20
1,1':4', 1"-TERPHENYL	0.41-0.98	6.0	32
1,1':3', 1"-TERPHENYL	0.41-1.00	7.8	29
1,1':2', 1"-TERPHENYL	0.38-0.99	14.6	32
BENZENE, 1,1'-ETHYLIDENEBIS-	0.70-1.00	0.4	6
BENZENE, 1,1'-METHYLENEBIS-	0.39-0.91	4.9	16

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, (PHENYLETHYL)-	0.71-0.99	0.2	6
BENZENE, 1,1',1"-METHYLIDYNETRIS-	0.42-0.99	0.8	8
BENZENE, PENTYL-	0.29-1.00	2.2	7
BENZENE, HEXYL-	0.30-0.93	1.8	6
BENZENE, OCTYL-	0.33-0.95	2.0	7
BENZENE, NONYL-	0.34-0.90	1.5	6
BENZENE, UNDECYL-	0.35-0.99	1.8	7
BENZENE, TRIDECYL-	0.36-0.96	1.6	7
BENZENE, TETRADECYL-	0.36-0.95	1.5	7
BENZENE, DODECYL-	0.35-0.97	1.7	7
1-ETHYL-3,5-DIMETHYL BENZENE	0.29-0.91	2.4	6
2-ETHYL-1,3-DIMETHYL BENZENE	0.38-0.93	1.6	6
BENZENE, 2-ETHYL-1,4-DIMETHYL-	0.33-0.92	1.1	6
BENZENE, 1-ETHYL-,2,4-DIMETHYL-	0.32-0.90	1.5	6
4-ETHYL-1,2-DIMETHYLBENZENE	0.31-0.90	1.6	6
BENZENE, 1-ETHYL-2,3-DIMETHYL-	0.69-1.00	0.1	5
BENZENE, 1,1'-(1,1,2,2-TETRAMETHYL-1,2-ETHANEDIYL)bis-	0.49-0.93	0.6	7
BENZENE, (1-METHYLENEPROPYL)-	0.38-0.94	1.2	6
BENZENE, (1-METHYL-1-PROPENYL)-,(E)-	0.36-0.91	1.3	6
BENZENE, (1-METHYL-1-PROPENYL)-, (Z)	0.42-0.97	1.5	6
BENZENE, 1-METHYL-2-PROPYL-	0.32-0.98	0.2	6
BENZENE, 1-METHYL-3-PROPYL-	0.29-0.98	0.3	6
BENZENE, 1-METHYL-4-PROPYLBENZENE	0.32-0.99	0.9	6
BENZENE,1,1',1"-(1-ETHANYL-2-YLIDENE)tris-	0.39-0.92	0.7	7
BENZENE, 1,1',1",1'"-METHANETETRAYLTETRAKIS-	0.57-0.97	0.4	9
BENZENE, 1,1',1",1'"-(1,2-ETHANEDIYLIDENE)TETRAKIS-	0.59-0.93	0.5	6
BENZENE, 1-ETHYL-4-(2 PHENYLETHYL)-	0.38-0.99	1.3	7
BENZENE, 1,2-DIMETHYL-3-PROPYL-	0.36-1.00	0.2	12
BENZENE, 1,2,3-TRIMETHYL-4-ETHYL-	0.37-0.94	0.1	7
BENZENE, 1,2,4-TRIMETHYL-3-ETHYL-	0.37-0.95	0.1	7

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, 1,2,4-TRIMETHYL-5-ETHYL-	0.38-0.97	0.1	7
1,1'-(1,2-ETHANEDIYL)BIS(4-ETHYL-) BENZENE	0.44-0.98	0.5	8
BENZENE, ETHENYL-	0.38-0.98	13.2	16
BENZENE, 1-ETHENYL-2-METHYL-	0.31-0.91	1.8	6
BENZENE, 1-ETHENYL-3-METHYL-	0.28-0.90	2.2	6
BENZENE, 1-ETHENYL-2-ETHYL-	0.30-0.98	0.5	9
BENZENE, 1-ETHENYL-3-ETHYL-	0.26-0.96	0.2	9
BENZENE, 1-ETHENYL-4-ETHYL-	0.33-0.99	0.3	9
BENZENE, 1-ETHENYL-4-METHYL-	0.36-0.93	0.9	6
BENZENE, (1-METHYLETHENYL)-	0.38-0.89	1.1	5
BENZENE, 1,3-DIETHENYL-	0.30-0.98	1.4	7
BENZENE, ETHYNYL-	0.35-0.88	0.4	5
BENZENE, 1-ETHENYL-4-(2-METHYLPROPYL)	0.34-0.95	1.9	7
BENZENE, 1-PROPENYL-,(Z)-	0.32-0.97	0.5	6
BENZENE, 1-PROPENYL-,(E)-	0.36-0.99	0.2	6
BENZENE, 1-ETHENYL-4-(1-METHYLETHENYL)-	0.28-0.99	2.7	7
BENZENE, 1-(1,1-DIMETHYLETHYL)-4-ETHENYL-	0.33-0.93	1.3	6
NAPHTHALENE	0.30-0.99	6.4	12
NAPHTHALENE, 1-METHYL-	0.31-0.97	0.8	7
NAPHTHALENE, 2-METHYL-	0.40-0.91	0.3	6
NAPHTHALENE, 1-ETHYL-	0.33-0.91	1.1	7
NAPHTHALENE, 1,2,3,4-TETRAHYDRO-	0.33-0.96	3.0	12
NAPHTHALENE, 2,6-DIMETHYL-	0.49-0.96	0.2	7
NAPHTHALENE, 1-PHENYL-	0.72-0.99	0.2	7
NAPHTHALENE, 1-NONYL-	0.34-0.92	1.5	8
NAPHTHALENE, 1-DECYL-	0.76-1.00	0.1	7
NAPHTHALENE, 1-BUTYL-	0.32-0.97	1.3	8
NAPHTHALENE, 1-HEXYL-	0.31-0.95	1.7	8
NAPHTHALENE, 2,7-DIMETHYL-	0.48-0.96	0.5	7
NAPHTHALENE, 1-HEXYL-1,2,3,4-TETRAHYDRO-	0.26-0.98	3.5	8
FLUORANTHENE	0.42-0.96	1.0	9
NAPHTHALENE, 1-PROPYL-	0.34-1.00	1.9	8
NAPHTHALENE, 2-ETHYL	0.35-0.92	0.6	7
1H-INDENE, 1-METHYL-	0.67-0.97	0.3	5

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1H-INDENE, 2-METHYL-	0.39-0.90	0.5	6
1H-INDENE, 1,2,3-TRIMETHYL-	0.48-0.92	0.5	6
3a,4,7,7a-TETRAHYDRODIMETHYL-4,7-METHANO-1H-INDENE	0.33-0.99	0.8	9
INDENE, 1-PHENYL-	0.43-0.99	1.0	8
BENZENE, 1,1',1''-(1-ETHENYL-2-YLIDENE)TRIS-	0.38-0.95	1.1	9
BENZENE, 1,1',1'',1'''-(1,2-ETHENEDIYLIDENE)TETRAKIS-	0.50-0.95	0.4	10
BENZENE, 1,1'-(1,2-ETHENEDIYL)BIS-, (Z)-	0.35-0.97	1.0	7
BENZENE, 1,1'-(1,2-ETHENEDIYL)BIS-, (E)-	0.71-0.96	0.2	6
BENZENE, 1,3-DIMETHOXY-5-(2-PHENYLETHENYL)-,(E)-	0.37-0.97	0.3	12
9H-FLUORENE	0.69-1.00	0.3	7
1H-INDENE	0.40-0.98	1.0	6
ANTHRACENE	0.71-0.97	0.1	7
PHENANTHRENE	0.43-0.99	1.0	8
CHRYSENE	0.54-0.97	0.4	9
PYRENE	0.45-1.00	0.9	9
ACENAPHTHYLENE, 1,2-DIHYDRO-	0.69-0.96	0.2	6
ACENAPHTHALENE	0.46-0.99	0.7	7
TRICYLCO(3.3.1.13,7)DECANE	0.66-1.00	0.1	5
BICYCLO(2.2.1)HEPT-2-ENE, 5-ETHENYL-	0.31-0.95	0.9	6
3,5,1,7-(1,2,3,4)BUTANETETRAYLNAPHTHALENE, DECAHYDRO-	0.66-0.96	0.1	6
1,3-DIMETHYLTRICYCLO[3.3.1.1(3,7)]DECANE	0.35-0.97	1.2	12
BICYCLO(2,2,1)HEPT-2-ENE,2-METHYL	0.37-0.94	0.6	5
BICYLCO(2,2,1)HEPT-2-ENE)5-ETHYL-	0.32-0.89	0.5	5
1H-INDENE, 2,3-DIHYDRO-	0.32-1.00	0.5	7
1,3-CYCLOHEXADIENE, 1-METHYL-4-(1-METHYLETHYL)-	0.34-0.94	0.5	6
1,4-CYCLOHEXADIENE, 1-METHYL-4-(1-METHYLETHYL)-	0.33-0.92	0.8	6
BICYCLO(2.2.1)HEPT-2-ENE	0.55-0.90	1.0	4

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZ(a)ANTHRACENE	0.44-0.96	0.9	9
NAPHTHACENE	0.64-0.97	0.1	9
7-ETHENYL-1,2,3,4,4a,4b,5,6,7,9,10-10a-DODECAHYDRO-1,4a,7-TRIMETHYL-1-PHENANTHRENECARBOXYLIC ACID	0.61-0.97	0.4	12
[1R-(1 alpha,4 abeta,4 balpha,7 alpha,10 aalpha)]-7ETHENYL-1,2,3,4,4a,4b,5,6,7,8,10,10a-DODECAHYDRO-1,4a,7-TRIMETHYL-1-PHENANTHRENECARBOXYLIC ACID	0.54-0.98	0.4	13
BICYCLO(2.2.1)HEPTANE, 2,2-DIMETHYL-3-METHYLENE-	0.50-0.92	0.2	5
BICYCLO(3.1.1)HEPT-2-ENE, 2,6,6-TRIMETHYL-	0.33-0.94	1.6	6
BICYCLO(3.1.1)HEPTANE, 6,6-DIMETHYL-2-METHYLENE	0.33-0.94	0.9	6
NITROUS OXIDE (N2O)	0.32-0.97	6.5	27
NITROGEN DIOXIDE (NO2)	0.70-1.00	4.2	28
OXYGEN	0.52-0.97	2.0	38
HYDROGEN	0.30-0.90	6.7	10
NITROGEN	0.50-0.99	1.4	37
CARBON MONOXIDE	0.55-0.85	1.2	6
CARBON DIOXIDE	0.56-1.00	0.6	39
SULFUR DIOXIDE	0.46-1.00	1.4	47
SULFUR TRIOXIDE	0.40-0.91	4.0	6
NITROGEN OXIDE (NO)	0.61-1.00	1.7	10
BROMINE	0.48-0.84	0.6	22
OZONE	0.31-0.94	3.7	5
PROPANAL	0.38-0.96	4.6	12
3-CYCLOHEXENE-1-CARBOXALDEHYDE	0.27-0.99	4.7	9

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
HEPTANAL	0.37-0.93	1.9	5
HEXANAL	0.37-0.96	2.9	5
OCTANAL	0.39-0.97	0.9	6
NONANAL	0.39-0.95	1.5	6
HEXANAL, 2-ETHYL-	0.72-0.99	0.2	4
ETHANEDIAL	0.65-0.92	0.1	3
HEXANAL, 2-METHYL-	0.40-0.91	1.3	5
HEXANAL, 3-METHYL-	0.39-0.91	3.3	5
2-PENTENAL, 2-METHYL-	0.39-0.95	3.2	5
2-HEXENAL, 2-ETHYL-	0.39-0.92	2.9	5
DECANAL	0.72-0.95	0.0	4
UNDECANAL	0.40-0.92	2.2	6
1-DODECANAL	0.74-0.94	0.1	4
TRIDECANAL	0.40-0.99	2.6	7
BUTANAL, 2-METHYL	0.39-0.91	2.2	6
3-METHYL-BUTANAL	0.41-0.92	2.4	6
2-PROPENAL	0.54-0.91	2.1	6
2-BUTENAL, (Z)-	0.29-0.98	2.1	6
trans-CROTONALDEHYDE	0.66-0.99	0.2	4
2-PROPENAL, 2-METHYL-	0.64-0.89	0.5	3
BENZENEACETALDEHYDE, alpha-METHYL-	0.42-1.00	0.2	6
BENZALDEHYDE, 2-METHYL-	0.34-1.00	0.6	7
BENZALDEHYDE, 4-METHYL-	0.68-0.98	0.6	5
BENZALDEHYDE	0.65-0.96	0.1	5
BENZALDEHYDE, 2-HYDROXY-	0.40-1.00	1.2	6
BENZALDEHYDE, 4-HYDROXY-	0.46-0.96	0.1	8
1,4-BENZENEDICARBOXALDEHYDE	0.53-0.99	0.6	6
BENZALDEHYDE, 3-METHYL-	0.36-0.97	0.4	6
1,3,5-TRIOXANE, 2,4,6-TRIMETHYL-	0.69-1.00	0.4	4
2-PROPANONE	0.67-0.97	0.6	9
2-BUTANONE	0.37-1.00	2.6	19
3-PENTANONE	0.42-0.96	1.1	10
2-PENTANONE, 4-METHYL-	0.33-0.96	3.3	11
2-PENTANONE, 3-METHYL-	0.29-0.87	0.1	5
3-HEPTANONE	0.39-0.95	0.1	5
4-HEPTANONE	0.40-0.96	0.1	5
3-HEXANONE	0.37-0.91	0.6	5
2-PENTANONE	0.67-0.89	0.3	3

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
2-BUTANONE, 3-METHYL-	0.33-0.98	5.1	5
2-HEXANONE	0.37-0.96	1.2	5
2-HEPTANONE	0.39-0.94	0.8	5
2-HEXANONE, 5-METHYL-	0.70-0.99	0.1	4
3-PENTEN-2-ONE, 4-METHYL-	0.67-0.97	0.1	4
2-BUTANONE, 3,3-DIMETHYL-	0.39-0.94	3.1	5
4-HEPTANONE, 2,6-DIMETHYL-	0.37-1.00	3.7	6
3-PENTANONE, 2,4-DIMETHYL-	0.36-0.90	0.6	5
2-PYRROLIDINONE	0.37-0.96	3.6	7
2-PYRROLIDINONE, 1-METHYL-	0.35-0.92	3.5	6
5-NONANONE	0.42-0.93	0.8	5
2-NONANONE	0.41-0.91	2.3	5
9,10-ANTHRACENEDIONE	0.62-0.95	0.9	7
2,4-PENTANEDIONE	0.39-0.97	3.7	6
2-CYCLOHEXEN-1-ONE, 3,5,5-TRIMETHYL-	0.68-0.97	4.5	10
CYCLOPENTANONE	0.36-0.97	4.5	10
CYCLOHEXANONE	0.37-0.89	0.9	5
2-OCTANONE	0.40-0.92	1.7	5
METHANONE, DIPHENYL-	0.70-0.95	0.1	6
ETHANONE, 1-PHENYL-	0.41-0.97	1.0	6
2-OXETANONE	0.35-0.90	2.0	6
2(3H)-FURANONE, DIHYDRO-	0.65-1.00	7.6	12
2-OXEPANONE	0.63-0.96	0.1	6
2(3H)-FURANONE, DIHYDRO-5-METHYL-	0.33-0.91	1.6	6
2-METHYL, 3-PENTANONE-	0.36-0.98	3.9	5
3-BUTEN-2-ONE, 3-METHYL	0.39-0.94	0.4	5
(1,1'-BICYCLOHEXYL)-2-ONE	0.31-0.95	1.1	7
2,5-CYCLOHEXADIENE-1,4-DIONE	0.57-0.93	0.1	5
2-OXETANONE, 4-METHYLENE-	0.43-0.91	1.4	6
ETHENONE	0.54-0.95	0.2	4
METHANOL	0.53-0.98	0.9	16
ETHANOL	0.53-0.99	1.3	43
1-PROPANOL	0.51-0.99	1.6	20
2-PROPANOL	0.54-1.00	0.6	22
1-BUTANOL	0.62-0.98	7.0	18
1-PROPANOL, 2-METHYL-	0.37-0.97	2.2	19

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
2-PROPANOL, 2-METHYL-	0.60-0.94	1.4	5
1-PENTANOL	0.47-1.00	2.5	13
2-PENTANOL	0.70-0.97	0.5	6
2-BUTANOL, 2-METHYL-	0.49-0.92	1.1	7
1-BUTANOL, 2-METHYL-	0.34-0.96	3.0	5
1-PROPANOL, 2,2-DIMETHYL-	0.70-0.98	0.2	6
1-HEXANOL	0.46-0.99	2.6	15
2-HEXANOL	0.38-0.97	2.1	5
1-PENTANOL, 2-METHYL-	0.37-0.94	1.7	5
1-PENTANOL, 3-METHYL-	0.35-0.95	1.5	5
3-PENTANOL, 3-METHYL-	0.43-0.87	0.1	4
3-PENTANOL	0.37-1.00	1.4	5
1-HEXANOL, 2-ETHYL-	0.70-0.94	0.5	4
1-HEXANOL, 2-METHYL-	0.37-0.95	3.8	5
1-BUTANOL, 3-METHYL-	0.27-0.91	4.8	8
2-BUTANOL, 3-METHYL-	0.34-0.99	0.9	5
1-HEPTANOL	0.71-0.97	0.4	4
2-HEPTANOL	0.40-0.95	2.3	5
1-HEXANOL, 5-METHYL-	0.49-0.95	0.3	5
2-PENTANOL, 4-METHYL-	0.71-0.97	0.5	6
1-OCTANOL	0.72-0.96	0.4	4
2-OCTANOL	0.38-0.92	1.0	5
1-NONANOL	0.73-0.95	0.5	4
2-NONANOL	0.37-0.89	3.1	5
1-DECANOL	0.73-0.95	0.5	4
1-UNDECANOL	0.41-0.97	2.3	6
1-NONANOL, 8-METHYL-	0.77-1.00	0.4	4
1-DODECANOL	0.74-1.00	0.2	5
1-TRIDECANOL	0.75-0.99	0.7	5
1-TETRADECANOL	0.75-0.98	0.2	5
1-PENTADECANOL	0.42-0.96	2.6	7
1-HEXADECANOL	0.76-0.97	0.1	5
1-HEPTADECANOL	0.77-0.97	0.4	5
1-OCTADECANOL	0.77-0.97	0.1	5
1-BUTANOL, 2-ETHYL-	0.72-0.92	0.3	3
1-EICOSANOL	0.78-0.96	0.3	5
1-NONADECANOL	0.42-1.00	0.5	8
CYCLOHEXANOL	0.46-1.00	0.8	6
CYCLOHEXANOL, 1-METHYL-	0.44-0.95	0.3	6

Table B.2. Vapor viscosity data used for model validation

Compound Name	Reduced Temperature Range	%AAD	Data points
CYCLOHEXANOL, 2-METHYL-, cis-	0.71-0.99	0.2	4
CYCLOHEXANOL, 2-METHYL-, trans-	0.71-0.99	0.2	4
CYCLOHEXANOL, 3-METHYL-, cis-	0.71-0.97	0.6	4
CYCLOHEXANOL, 3-METHYL-, trans-	0.70-0.97	0.2	4
CYCLOHEXANOL, 4-METHYL-, cis-	0.71-0.98	0.2	4
CYCLOHEXANOL, 4-METHYL-, trans-	0.71-0.98	0.1	4
cyclohexanol, 5-methyl-2-1(1-methylethyl)-[1R-{1 alpha, 2-beta, 5 alpha}]	0.48-1.00	0.4	6
STIGMAST-5-EN-3-OL,(3beta)-	0.43-0.98	1.0	9
1-NAPHTHALENEMETHANOL, DECAHYDRO-5-(5-HYDROXY-3-METHYL-3-PENTENYL)-1,4a-DIMETHYL-6-METHYLENE-, [1S-[1Alpha,4aAlpha,5Alpha(E),8aBeta]]	0.48-0.98	0.1	8
Alpha,Alpha,4-TRIMETHYL-3-CYCLOHEXENE-1-METHANOL	0.46-0.97	0.3	8
CYCLOHEXANOL, 1-METHYL-4-(1-METHYLETHENYL)	0.46-0.98	0.8	8
1-NONANOL, 2-BUTYL-	0.40-0.93	0.1	8
1-UNDECANOL, 2-METHYL-	0.40-0.95	0.1	8
2-FURANMETHANOL, TETRAHYDRO-	0.71-0.96	1.3	8
2-PROPEN-1-OL	0.68-0.91	0.3	3
BENZENEMETHANOL, alpha,alpha-DIMETHYL-	0.47-0.99	0.5	6
1-OCTANOL, 2-BUTYL	0.29-0.98	0.4	9
PHENOL, 2,3-DIMETHYL-	0.48-0.98	0.4	6
PHENOL, 2,4-DIMETHYL	0.68-0.97	0.0	5
PHENOL, 2,5-DIMETHYL-	0.49-0.90	1.2	5
PHENOL, 2,6-DIMETHYL-	0.46-1.00	0.7	6
PHENOL, 3,4-DIMETHYL-	0.46-0.97	1.1	6
PHENOL, 3,5-DIMETHYL-	0.47-0.99	0.2	6
2-PROPYN-1-OL	0.67-0.98	0.3	4
BENZENEMETHANOL	0.36-0.93	0.6	6
PHENOL	0.29-0.97	5.1	24
PHENOL, 2-METHYL-	0.44-0.99	7.3	11
PHENOL, 3-METHYL-	0.67-0.97	0.4	5
PHENOL, 4-METHYL-	0.67-0.97	0.4	5
PHENOL, 2-ETHYL-	0.38-0.96	0.2	6
1,4-BENZENEDIOL	0.54-0.99	0.6	7
PHENOL, 4-ETHYL-	0.44-0.97	0.6	6
PHENOL, 4-(1,1-DIMETHYLETHYL)-	0.51-0.98	0.1	6
PHENOL, 4,4'-(1-METHYLETHYLIDENE)bis-	0.34-0.99	12.8	7
PHENOL, NONYL	0.36-0.99	1.5	

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1,2-ETHANEDIOL	0.36-0.93	0.2	6
ETHANOL, 2,2'-OXYBIS-	0.35-0.97	4.6	19
ETHANOL, 2,2'-(1,2-ETHANEDIYLBIS(OXY))BIS-	0.26-0.98	15.8	26
ETHANOL, 2,2'-(OXYBIS(2,1-ETHANEDIYLOXY))BIS-	0.76-0.95	8.9	10
1,2-PROPANEDIOL	0.34-0.98	2.5	14
1,3-PROPANEDIOL	0.34-0.96	1.2	7
PROPANOL, OXYBIS-	0.76-0.99	0.3	4
1,3-PROPANEDIOL, 2,2-DIMETHYL-	0.64-0.95	0.2	4
2-BUTYNE-1,4-DIOL	0.48-0.90	1.5	5
PROPANOL,((1-METHYL-1,2-ETHANEDIYL)bis(oxy))bis-	0.34-0.97	5.0	6
1,3-PROPANEDIOL, 2-METHYL-	0.26-0.91	1.0	6
1,2-BUTANEDIOL	0.32-0.96	3.8	6
1,3-BUTANEDIOL	0.29-0.95	2.4	6
2,4-PENTANEDIOL, 2-METHYL-	0.36-0.93	2.9	8
1,2,3-PROPANETRIOL	0.33-0.99	4.4	19
1,2,3-BUTANETRIOL	0.37-0.95	0.3	9
1,2,4-BUTANETRIOL	0.39-0.99	2.5	9
1,2-BENZENEDIOL, 4-(1,1-DIMETHYLETHYL-)	0.43-0.91	1.8	6
1,3-PENTANEDIOL, 2,2,4-TRIMETHYL	0.48-0.97	1.3	6
1,3-PENTANEDIOL, 2-METHYL	0.38-0.94	0.9	10
2,3-BUTANEDIOL	0.46-0.92	1.8	5
2-BUTENE-1,4-DIOL, (Z)-	0.42-0.89	1.7	5
2-BUTENE-1,4-DIOL, (E)-	0.45-0.92	1.1	5
1,4-BUTANEDIOL	0.44-0.98	2.1	9
1,5-PENTANEDIOL	0.38-1.00	2.7	10
1,6-HEXANEDIOL	0.46-0.97	3.1	9
1,2-BENZENEDIOL	0.49-0.98	1.5	7
1,3-BENZENEDIOL	0.47-1.00	2.0	8
1,3-PROPANEDIOL, 2,2-BIS(HYDROXYMETHYL)-	0.81-0.99	0.2	5
1,3-PROPANEDIOL, 2-ETHYL-2-(HYDROXYMETHYL)-	0.79-0.96	0.3	5
1,2,3-BENZENETRIOL	0.49-0.97	1.3	7
D-GLUCITOL	0.42-0.93	2.7	8
FORMIC ACID	0.47-0.99	1.3	13

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
ACETIC ACID	0.46-0.97	4.5	24
PROPANOIC ACID	0.42-0.99	1.7	14
DECANOIC ACID	0.42-1.00	3.1	7
ETHANEDIOIC ACID	0.58-0.97	0.8	7
BUTANOIC ACID	0.44-0.93	1.3	12
BUTANOIC ACID, 2-METHYL-, (+ -)	0.70-0.95	0.2	4
PENTANOIC ACID	0.37-0.97	0.2	6
NONANOIC ACID	0.40-0.90	1.8	6
PROPANOIC ACID, 2-METHYL-	0.38-0.88	1.3	5
BUTANOIC ACID, 3-METHYL-	0.39-0.92	0.2	5
HEXANOIC ACID	0.41-0.90	0.3	5
HEXANOIC ACID, 2-METHYL-	0.35-0.92	0.3	8
1,4-CYCLOHEXANEDICARBOXYLIC ACID, trans-	0.66-0.98	0.8	8
OCTANOIC ACID	0.42-0.93	2.1	6
UNDECANOIC ACID	0.41-0.98	2.6	7
CYCLOPENTANEACETIC ACID	0.41-0.97	0.1	6
PROPANOIC ACID, 2,2'-OXYBIS-	0.58-1.00	0.6	5
DODECANOIC ACID	0.43-0.98	2.1	7
TRIDECANOIC ACID	0.42-0.96	3.1	7
TETRADECANOIC ACID	0.43-0.95	2.2	7
HEXADECANOIC ACID	0.43-0.93	0.4	7
2-BUTENOIC ACID, (Z)-	0.45-1.00	1.2	6
2-BUTENOIC ACID, (E)-	0.52-0.91	0.4	5
OCTANOIC ACID, 2-METHYL	0.35-0.97	0.1	9
OCTADECANOIC ACID	0.43-0.99	0.1	8
2-PROPENOIC ACID	0.45-0.93	11.4	12
2-PROPENOIC ACID, 2-METHYL-	0.44-0.97	0.4	6
9-OCTADECENOIC ACID(Z)-	0.37-0.91	0.3	7
9,12-OCTADECADIENOIC ACID(Z,Z)-	0.35-0.91	0.5	7
BENZOIC ACID	0.53-0.93	0.4	6
BENZOIC ACID, 2-METHYL-	0.50-1.00	1.5	7
BENZOIC ACID, 4-METHYL-	0.59-0.94	0.5	6
BENZOIC ACID, 2-HYDROXY-	0.58-0.96	0.4	6
HEXANEDIOIC ACID	0.53-0.95	1.2	7
2-BUTENEDIOIC ACID (Z)-	0.52-0.95	0.9	6
1,2-BENZENEDICARBOXYLIC ACID	0.80-0.98	0.2	5

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
ETHANEPEROXOIC ACID	0.49-0.89	55.2	9
ACETIC ACID, ANHYDRIDE	0.33-0.98	3.2	22
PROPANOIC ACID, ANHYDRIDE	0.37-0.98	9.1	12
BUTANOIC ACID, ANHYDRIDE	0.31-0.93	0.1	6
PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4a,5,6,9,10,10a-DECAHYDRO-1,4a-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1Alpha,4aBeta,10aAlpha)]-	0.56-0.97	0.8	12
2,5-FURANDIONE, DIHYDRO-	0.49-0.93	4.1	14
2H-PYRAN-2,6(3H)-DIONE, DIHYDRO-	0.39-0.95	0.4	8
1,3-ISOBENZOFURANDIONE	0.70-0.95	0.5	5
2,5-FURANDIONE	0.45-0.92	1.0	6
5-ISOBENZOFURANCARBOXYLIC ACID, 1,3-DIHYDRO-1,3-DIOXO-	0.75-0.98	0.2	8
FORMIC ACID, METHYL ESTER	0.62-0.92	0.2	4
FORMIC ACID, ETHYL ESTER	0.54-0.98	2.6	10
FORMIC ACID, PROPYL ESTER	0.65-0.93	0.3	4
FORMIC ACID, BUTYL ESTER	0.54-0.98	0.6	6
FORMIC ACID, 2-METHYLPROPYL ESTER	0.67-0.90	0.4	4
FORMIC ACID, PENTYL ESTER	0.35-0.90	0.2	5
FORMIC ACID, OCTYL ESTER	0.36-0.95	0.1	6
FORMIC ACID, NONYL ESTER	0.37-0.88	0.3	5
FORMIC ACID, DECYL ESTER	0.37-0.99	0.2	6
FORMIC ACID, ETHENYL ESTER	0.40-0.88	0.8	4
ACETIC ACID, METHYL ESTER	0.82-0.97	0.1	3
ACETIC ACID, ETHYL ESTER	0.36-1.00	7.8	16
ACETIC ACID, PROPYL ESTER	0.68-0.91	4.3	6
ACETIC ACID, BUTYL ESTER	0.35-0.97	4.5	8
ACETIC ACID, 2-METHYLPROPYL ESTER	0.31-0.98	17.6	21
1-BUTANOL, 3-METHYL-, ACETATE	0.33-0.88	9.8	9
ACETIC ACID, 2-PROPENYL ESTER	0.68-0.90	0.4	3
ACETIC ACID, 1-METHYLETHYL ESTER	0.68-0.92	0.4	3
ACETIC ACID, 1-METHYLPROPYL ESTER	0.69-0.90	0.4	3
ACETIC ACID, ETHENYL ESTER	0.35-0.98	2.7	15

Table B2. Vapor viscosity data used for external validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
PROPANOIC ACID, METHYL ESTER	0.66-0.94	4.4	7
PROPANOIC ACID, ETHYL ESTER	0.54-0.92	1.5	13
PROPANOIC ACID, PROPYL ESTER	0.70-0.91	5.9	6
PROPANOIC ACID, BUTYL ESTER	0.31-1.00	8.8	9
BUTANOIC ACID, PROPYL ESTER	0.30-1.00	10.1	25
PROPANOIC ACID, ETHENYL ESTER	0.67-0.95	0.3	6
BUTANOIC ACID, METHYL ESTER	0.68-0.90	0.2	3
BUTANOIC ACID, ETHYL ESTER	0.69-0.90	0.4	3
PROPANOIC ACID, 2-METHYL-, PROPYL ESTER	0.35-0.97	3.1	10
2-PROPENOIC ACID, METHYL ESTER	0.51-1.00	1.5	13
ACRYLIC ACID, ETHYL ESTER	0.53-1.00	3.2	12
2-PROPENOIC ACID, PROPYL ESTER	0.48-0.99	2.0	5
NONANOIC ACID, BUTYL ESTER	0.35-0.98	4.7	6
PENTANOIC ACID, BUTYL ESTER	0.29-0.93	6.4	6
BUTANOIC ACID, 3-METHYL-, ETHYL ESTER	0.30-0.92	3.0	5
2-PROPENOIC ACID, 2-METHYL-, METHYL ESTER	0.49-0.97	3.2	11
METHACRYLIC ACID, ETHYL ESTER	0.68-0.99	0.3	4
1,2-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.82-0.99	17.2	8
1,2-BENZENEDICARBOXYLIC ACID, DIISOOCTYL ESTER	0.26-0.99	2.0	9
ACETIC ACID, PENTYL ESTER	0.70-0.99	1.3	8
ACETIC ACID, 2-ETHYLHEXYL ESTER	0.73-0.98	0.1	4
ACETIC ACID, PHENYLMETHYL ESTER	0.32-0.94	0.2	6

Table B.3. Comparison of vapor viscosity predictions for selected compounds

Compound name	Reduced Temperature Range	Lucas * Method (%AAD)	SVRC-QSPR Model (%AAD)
Pentane	0.64-0.98	1.7	0.3
Cyclohexane	0.58-0.94	2.9	0.4
Sulfur Dioxide	0.58-0.98	1.9	0.6

APPENDIX C

THE SVRC-QSPR MODEL FOR SURFACE TENSIONS: DATABASE USED FOR MODEL DEVELOPMENT AND VALIDATION

Table C1 Surface tension data used in model development

Compound Name	Reduced Temperature Range	Data points	%AAD	Reference
ETHANE	0.39-0.97	21	1.8	[1]
PROPANE	0.52-0.98	16	1.6	[1]
BUTANE	0.55-0.74	13	1.0	[1]
HEXANE	0.54-0.98	28	1.0	[1]
HEPTANE	0.52-0.93	30	2.0	[1]
PENTANE, 2,3-DIMETHYL-	0.45-0.66	15	0.9	[1]
OCTANE	0.41-0.88	31	2.5	[1]
CIS-DECALIN	0.35-0.64	27	2.2	[1]
TRANS-DECALIN	0.35-0.66	26	1.6	[1]
2-BUTENE, 2-METHYL-	0.43-0.75	22	0.8	[1]
CYCLOPENTENE	0.49-0.64	16	2.3	[1]
CYCLOHEXENE	0.43-0.62	30	0.8	[1]
BENZENE, METHYL-	0.46-0.63	11	0.4	[1]
BENZENE, 1,2-DIMETHYL-	0.43-0.59	11	0.2	[1]
BENZENE, 1,3,5-TRIMETHYL-	0.40-0.68	21	1.8	[1]
BIPHENYL	0.48-0.81	13	1.0	[1]
1,1':4', 1"-TERPHENYL	0.55-0.74	15	2.0	[1]
1,1':3', 1"-TERPHENYL	0.41-0.74	20	1.4	[1]
1,1':2', 1"-TERPHENYL	0.41-0.73	18	2.0	[1]
BENZENE, 1,1'-METHYLENEBIS-	0.40-0.48	12	2.4	[1]
SULFUR TRIOXIDE	0.60-0.96	13	3.0	[1]
3-PENTANONE	0.50-0.92	17	1.8	[1]
3-HEXANONE	0.51-0.62	13	0.6	[1]
CYCLOHEXANONE	0.44-0.55	12	1.5	[1]
METHANOL	0.54-0.97	23	1.0	[1]
ETHANOL	0.53-0.96	23	1.8	[1]
1-BUTANOL	0.49-0.73	20	1.7	[1]
1-HEXANOL	0.47-0.64	11	0.8	[1]
2-HEXANOL	0.48-0.71	15	0.5	[1]
1-PENTANOL, 2-METHYL-	0.46-0.68	14	0.9	[1]
1-PENTANOL, 3-METHYL-	0.46-0.70	16	2.4	[1]
2-PENTANOL, 4-METHYL-	0.49-0.71	16	0.7	[1]
1-NONANOL	0.41-0.56	12	0.5	[1]
PHENOL, 3-METHYL-	0.41-0.64	14	0.8	[1]
FORMIC ACID	0.49-0.59	12	0.6	[1]
PROPANOIC ACID, 2-METHYL-	0.48-0.67	15	2.9	[1]
DODECANOIC ACID	0.43-0.56	17	0.9	[1]
TETRADECANOIC ACID	0.43-0.55	17	1.1	[1]
HEXADECANOIC ACID	0.43-0.54	13	0.3	[1]
ACETIC ACID, ANHYDRIDE	0.48-0.53	14	0.4	[1]

Table C1. Surface tension data used in model development (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points	Reference
ACETIC ACID, PROPYL ESTER	0.52-0.68	0.4	12	[1]
ACETIC ACID, 2-METHYLPROPYL ESTER	0.50-0.68	2.4	14	[1]
PROPANOIC ACID, ETHYL ESTER	0.52-0.65	0.6	11	[1]
BUTANOIC ACID, METHYL ESTER	0.51-0.92	1.9	14	[1]
BUTANOIC ACID, ETHYL ESTER	0.49-0.69	0.6	11	[1]
ACETIC ACID, PENTYL ESTER	0.48-0.60	0.3	11	[1]
ACETIC ACID, HEXYL ESTER	0.47-0.58	0.6	12	[1]
BENZOIC ACID, PHENYLMETHYL ESTER	0.36-0.59	2.7	11	[1]
BENZOIC ACID, METHYL ESTER	0.41-0.68	0.5	15	[1]
BENZOIC ACID, ETHYL ESTER	0.39-0.68	0.8	16	[1]
CARBONIC ACID, DIETHYL ESTER	0.50-0.63	0.4	16	[1]
ETHANEDIOIC ACID, DIETHYL ESTER	0.41-0.74	1.8	19	[1]
PROPANEDIOIC ACID, DIETHYL ESTER	0.39-0.68	2.6	14	[1]
ETHANE, 1,1'-OXYBIS-	0.62-0.91	1.3	16	[1]
ETHANE, 1,1-DIETHOXY-	0.53-0.70	0.7	11	[1]
OXIRANE	0.48-0.63	0.6	11	[1]
BENZENE, METHOXY-	0.44-0.66	0.8	16	[1]
BENZENE, ETHOXY-	0.39-0.69	2.5	14	[1]
BENZENE, 1,1'-OXYBIS-	0.38-0.68	1.8	13	[1]
FURAN, TETRAHYDRO-	0.51-0.65	0.5	17	[1]
PROPANE, 1,2 DICHLORO-	0.50-0.65	1.2	11	[1]
BENZENE, 1,4-DICHLORO-	0.48-0.65	0.5	11	[1]
METHANE, DICHLORODIFLUORO-	0.71-0.90	3.4	25	[1]
METHANE, TRICHLOROFLUORO-	0.50-0.78	2.6	30	[1]
ETHANE, 1,2-DICHLORO-1,1,2,2-TETRAFLUORO-	0.65-0.83	0.9	18	[1]
ETHANE, 1,2-DIBROMO-1,1,2,2-TETRAFLUORO-	0.60-0.75	1.5	11	[1]
METHANE, DIFLUORO-	0.76-0.93	1.9	12	[1]
ETHANE, 1,1,1-TRIFLUORO-	0.79-0.92	1.3	19	[1]
ETHANE, PENTAFLUORO-	0.69-0.98	0.7	21	[1]
ETHANE, IODO-	0.51-0.62	1.1	11	[1]
BENZENE, IODO-	0.40-0.59	0.6	12	[1]
ETHANE, 1,1-DICHLORO-2,2,2-TRIFLUORO-	0.55-0.93	0.5	18	[1]

Table C1. Surface tension data used in model development (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points	Reference
1-PROPANAMINE, N-PROPYL-	0.52-0.66	0.6	14	[1]
ETHANAMINE, N-ETHYL-	0.58-0.66	1.3	12	[1]
HYDRAZINE	0.42-0.54	2.1	18	[1]
ETHANOL, 2-AMINO-	0.43-0.53	0.3	13	[1]
BENZENEMETHANAMINE	0.43-0.53	0.6	17	[1]
BENZENAMINE, 2-METHYL-	0.38-0.66	2.3	14	[1]
BENZENAMINE, 3-METHYL-	0.42-0.60	1.1	16	[1]
BENZENAMINE, 4-METHYL-	0.46-0.70	1.5	13	[1]
QUINOLINE	0.36-0.86	2.7	14	[1]
METHANE, NITRO-	0.47-0.64	0.9	23	[1]
ETHANE, NITRO-	0.46-0.65	1.1	20	[1]
PROPANE, 1-NITRO-	0.45-0.60	1.4	12	[1]
PROPANE, 2-NITRO-	0.46-0.61	0.9	13	[1]
HYDROCYANIC ACID	0.57-0.65	0.3	15	[1]
BENZENE, 1-METHYL-2-NITRO-	0.38-0.65	2.8	21	[1]
BENZENE, 1-METHYL-4-NITRO-	0.44-0.66	1.5	22	[1]
PYRIDINE	0.44-0.63	1.5	13	[1]
BENZENAMINE, N,N-DIMETHYL-	0.41-0.65	1.6	14	[1]
ETHANE, 1,1'-THIOBIS-	0.51-0.65	0.4	14	[1]
THIOPHENE	0.50-0.58	1.2	18	[1]
ETHANE, 1,1'-OXYBIS(2-CHLORO-	0.43-0.54	0.7	12	[1]
BENZENE, NITRO-	0.39-0.66	2.6	26	[1]
BENZENE, 1-METHOXY-2-NITRO-	0.38-0.59	1.2	13	[1]
SILANE, TRICHLORO-	0.55-0.65	2.2	23	[1]
SILANE, TETRACHLORO-	0.54-0.65	2.0	14	[1]
HEXAMETHYLDISILOXANE	0.43-0.69	2.7	50	[1]
CYCLOTETRASILOXANE, OCTAMETHYL-	0.50-0.55	0.9	15	[1]
WATER-D2	0.43-0.76	1.4	24	[1]
DOTRIACONTANE	0.41-0.49	0.4	12	[1]
DODECANOIC ACID, METHYL ESTER	0.40-0.51	0.9	12	[1]
PROPANE, 1,3-DICHLORO-	0.48-0.60	0.5	14	[1]
ETHANE, 1,1,1,2-TETRAFLUORO-	0.68-0.97	1.4	28	[1]
ETHANE, 1,1,2-TRICHLORO-1,2,2-TRIFLUORO-	0.56-0.76	0.9	26	[1]
1-HEXANAMINE	0.42-0.66	4.8	16	[1]
3-BUTENENITRILE	0.49-0.62	0.2	15	[1]

Table C1. Surface tension data used in model development (contd.)

Compound Name	Reduced Temperature Range	Data points	%AAD	Reference
FORMAMIDE	0.38-0.45	0.5	12	[1]
ETHANOL, 2-METHOXY-	0.51-0.64	0.8	13	[1]
ETHANOL, 2-ETHOXY-	0.52-0.63	0.8	15	[1]
ETHANOL, 2-BUTOXY-	0.46-0.55	4.1	11	[1]
TRISILOXANE, OCTAMETHYL-	0.52-0.58	1.3	11	[1]
DIMETHYL SUCCINATE	0.44-0.68	1.9	17	[1]
BENZENAMINE, 4-CHLORO-	0.46-0.61	0.2	15	[1]
SULFUROUS ACID, DIETHYL ESTER	0.45-0.58	1.4	17	[1]
HYDROGEN	0.39-0.71	0.4	9	[1]
SILANE, TRICHLOROMETHYL-	0.57-0.76	1.1	11	[1]
SILANE, CHLOROTRIMETHYL-	0.55-0.65	2.6	11	[1]
BENZENE, 1,2-DICHLORO-4-NITRO-	0.42-0.63	1.8	10	[1]
TETRASILOXANE, DECAMETHYL-	0.49-0.56	0.5	15	[1]
PROPANENITRILE, 2-HYDROXY-	0.45-0.57	0.2	13	[1]
SULFURIC ACID, DIETHYL ESTER	0.38-0.54	1.5	12	[1]
PARALDEHYDE	0.49-0.64	1.5	10	[2]
BENZALDEHYDE	0.41-0.54	0.4	10	[2]
2-FURALDEHYDE	0.42-0.56	2.4	10	[2]
ACETIC ANHYDRIDE	0.43-0.65	2.1	11	[2]
BUTYL ALCOHOL	0.50-0.66	0.4	10	[2]
ISOBUTYL ALCOHOL	0.53-0.70	3.4	10	[2]
PENTANOL	0.48-0.64	0.2	10	[2]
3-METHYL-1-BUTANOL	0.49-0.65	0.6	10	[2]
2-PENTANOL	0.51-0.67	2.7	10	[2]
2-METHOXYETHANE	0.50-0.66	1.9	10	[2]
2-BUTOXYETHANE	0.45-0.59	0.8	10	[2]
1-NONANOL	0.42-0.56	0.8	10	[2]
1-DECANOL	0.41-0.54	1.1	10	[2]
ETHYL ACETATE	0.54-0.71	0.3	10	[2]
PROPYL ACETATE	0.52-0.68	1.5	10	[2]
BUTYL ACETATE	0.49-0.65	1.2	10	[2]
ISOBUTYL ACETATE	0.51-0.67	1.3	10	[2]
SEC-BUTYL ACETATE	0.51-0.67	1.6	10	[2]
1-PENTYL ACETATE	0.47-0.62	0.6	10	[2]
3-METHYLBUTYL ACETATE	0.51-0.67	1.8	10	[2]
HEXYL ACETATE	0.46-0.60	0.7	10	[2]

Table C1. Surface tension data used in model development (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points	Reference
METHYL FORMATE	0.60-0.79	0.8	10	[2]
BUTYL FORMATE	0.51-0.67	0.5	10	[2]
1-PENTYL FORMATE	0.49-0.65	0.3	10	[2]
HEXYL FORMATE	0.47-0.62	0.3	9	[2]
PROPYL PROPIONATE	0.53-0.70	2.6	10	[2]
BUTYL PROPIONATE	0.48-0.63	0.9	10	[2]
CYCLOPENTANONE	0.45-0.60	0.6	11	[2]
CYCLOHEXANONE	0.43-0.57	3.2	11	[2]
ETHYLBENZENE	0.46-0.61	0.2	10	[2]
PROPYLBENZENE	0.44-0.59	0.9	10	[2]
CUMENE	0.45-0.59	0.6	10	[2]
BUTYLBENZENE	0.43-0.57	0.9	10	[2]
ISOBUTYLBENZENE	0.44-0.57	0.3	10	[2]
SEC-BUTYLBENZENE	0.43-0.56	0.5	10	[2]
TERT-BUTYLBENZENE	0.43-0.57	0.6	10	[2]
PENTYLBENZENE	0.42-0.55	0.3	10	[2]
1-PHENYLHEXANE	0.41-0.54	0.5	10	[2]
O-XYLENE	0.45-0.59	0.2	10	[2]
M-XYLENE	0.46-0.61	0.2	10	[2]
O-ETHYLTOLUENE	0.44-0.57	0.4	10	[2]
M-ETHYLTOLUENE	0.45-0.59	1.3	10	[2]
P-ETHYLTOLUENE	0.44-0.58	1.0	10	[2]
O-DIETHYLBENZE	0.42-0.56	0.4	10	[2]
M-DIETHYLBENZE	0.43-0.56	1.2	10	[2]
P-DIETHYLBENZENE	0.43-0.57	0.7	10	[2]
2-METHYL-1-PENTENE	0.48-0.64	0.3	11	[2]
4-METHYL-2-PENTENE	0.50-0.68	0.6	11	[2]
3-METHYL-1-PENTENE	0.49-0.66	1.8	11	[2]
3-METHYL-3-PENTENE	0.50-0.67	0.3	11	[2]
2-HEXANOL	0.49-0.66	0.1	11	[2]
1-OCTENE	0.50-0.66	0.4	9	[2]
1-NONENE	0.48-0.63	0.2	9	[2]
1-DECENE	0.46-0.61	0.2	9	[2]
1-UNDECENE	0.44-0.59	0.2	10	[2]
1-DODECENE	0.43-0.57	0.1	10	[2]
1-TRIDECENE	0.42-0.55	0.2	10	[2]
1-TETRADECENE	0.41-0.54	0.2	10	[2]
1-PENTADECENE	0.40-0.53	0.2	10	[2]
3-ETHYLPENTANE	0.47-0.65	0.8	11	[2]
2-METHYLHEXANE	0.48-0.69	1.2	12	[2]
3-METHYLHEXANE	0.47-0.68	1.2	12	[2]

Table C1. Surface tension data used in model development (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points	Reference
3-ETHYL, 2-METHYLPENTANE	0.50-0.66	0.7	11	[2]
3-ETHYL, 3-METHYLPENTANE	0.49-0.65	0.9	11	[2]
2-BUTANONE	0.54-0.66	2.6	9	[2]
2-PENTANONE	0.51-0.65	2.6	10	[2]
3-HEXANONE	0.49-0.62	2.1	10	[2]
4-HEPTANONE	0.47-0.59	1.3	10	[2]
DIFLUOROMETHANE (R-32)	0.78-0.95	2.0	13	[4]
CHLOROTETRAFLUOROETHANE (R-124)	0.70-0.87	1.2	15	[5]
MONOCHLORODIFLUOROETHANE (R-142B)	0.67-0.83	0.8	16	[4]
DIFLUOROETHANE (R-152A)	0.71-0.89	0.4	19	[4]
PROPANE	0.74-0.99	1.2	30	[6]
ISOBUTANE	0.67-0.98	0.8	29	[6]

Table C2. Surface tension data used for model validation

Compound Name	Reduced Temperature Range	%AAD	Data points
METHANE	0.47-1.00	11.5	18
ETHANE	0.39-0.99	4.2	36
PROPANE	0.50-0.99	21.2	36
PROPANE, 2-METHYL-	0.50-0.72	0.8	9
BUTANE	0.48-0.75	2.6	30
PENTANE	0.54-0.67	0.3	11
BUTANE, 2-METHYL-	0.55-0.66	0.3	12
PROPANE, 2,2-DIMETHYL-	0.59-0.89	1.8	11
HEXANE	0.54-0.97	3.9	29
PENTANE, 2-METHYL-	0.55-0.67	0.6	8
PENTANE, 3-METHYL-	0.54-0.66	0.2	8
BUTANE, 2,2-DIMETHYL-	0.56-0.64	0.7	6
BUTANE, 2,3-DIMETHYL-	0.55-0.63	0.4	6
HEPTANE	0.52-0.93	0.9	31
HEXANE, 2-METHYL-	0.46-0.69	0.8	16
HEXANE, 3-METHYL-	0.45-0.68	0.5	17
PENTANE, 3-ETHYL-	0.45-0.67	0.6	25
PENTANE, 2,2-DIMETHYL-	0.29-0.90	1.1	33
PENTANE, 2,3-DIMETHYL-	0.45-0.66	0.5	17
PENTANE, 2,4-DIMETHYL-	0.47-0.68	0.7	14
PENTANE, 3,3-DIMETHYL-	0.45-0.66	0.6	24
BUTANE, 2,2,3-TRIMETHYL-	0.47-0.88	2.9	13
OCTANE	0.41-0.89	0.8	43
HEPTANE, 2-METHYL-	0.49-0.67	1.1	25
HEPTANE, 3-METHYL-	0.49-0.66	0.9	23
HEPTANE, 4-METHYL-	0.49-0.66	0.6	22
HEXANE, 3-ETHYL-	0.48-0.66	0.7	23
HEXANE, 2,2-DIMETHYL-	0.50-0.68	1.0	23
HEXANE, 2,3-DIMETHYL-	0.49-0.66	0.5	23
HEXANE, 2,4-DIMETHYL-	0.49-0.67	0.6	23
HEXANE, 2,5-DIMETHYL-	0.50-0.68	0.9	23
HEXANE, 3,3-DIMETHYL-	0.49-0.66	0.7	23
HEXANE, 3,4-DIMETHYL-	0.48-0.66	0.8	23
PENTANE, 3-ETHYL-2-METHYL-	0.48-0.66	0.6	23
PENTANE, 3-ETHYL-3-METHYL-	0.47-0.65	0.5	12
PENTANE, 2,2,3,TRIMETHYL-	0.49-0.66	0.9	14
PENTANE, 2,2,4-TRIMETHYL-	0.50-0.67	0.5	14
PENTANE, 2,3,3-TRIMETHYL-	0.48-0.65	0.8	23
PENTANE, 2,3,4-TRIMETHYL-	0.48-0.66	0.7	23
BUTANE, 2,2,3,3-TETRAMETHYL-	0.52-0.90	3.0	13
NONANE	0.48-0.66	0.8	12

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
HEXANE, 2,2,5-TRIMETHYL-	0.48-0.59	0.3	7
HEPTANE, 3,3,5-TRIMETHYL-	0.27-0.90	1.5	14
HEXANE,2,4,4-TRIMETHYL-	0.47-0.57	0.8	8
PENTANE, 3,3-DIETHYL-	0.45-0.55	0.1	8
PENTANE, 2,2,3,3,-TETRAMETHYL-	0.45-0.55	0.3	15
PENTANE, 2,2,3,4-TETRAMETHYL-	0.46-0.56	0.4	16
PENTANE, 2,2,4,4-TETRAMETHYL-	0.48-0.58	0.2	16
PENTANE, 2,3,3,4-TETRAMETHYL-	0.45-0.55	0.5	8
TETRACOSANE, 2,6,10,15,19,23-HEXAMETHYL-	0.27-0.77	17.4	11
DECANE	0.46-0.64	1.0	12
HEXANE, 2,2,3,3-TETRAMETHYL-	0.35-0.90	2.6	14
HEXANE, 2,2,5,5-TETRAMETHYL-	0.45-0.90	1.1	11
UNDECANE	0.44-0.62	0.8	12
DODECANE	0.43-0.60	0.8	12
TRIDECANE	0.41-0.63	0.8	35
TETRADECANE	0.41-0.61	1.0	30
PENTADECANE	0.40-0.60	1.6	32
HEXADECANE	0.41-0.59	1.3	33
HEPTADECANE	0.40-0.53	1.7	27
OCTADECANE	0.39-0.53	1.3	32
NONADECANE	0.39-0.52	1.5	38
OCTANE, 2,2-DIMETHYL-	0.37-0.89	1.3	11
EICOSANE	0.38-0.51	1.3	38
HENEICOSANE	0.38-0.85	3.8	12
DOCOSANE	0.37-0.85	4.7	12
TRICOSANE	0.40-0.85	5.3	9
TETRACOSANE	0.40-0.85	6.9	9
PENTACOSANE	0.36-0.85	3.0	12
HEXACOSANE	0.36-0.85	3.7	19
HEPTACOSANE	0.40-0.85	7.8	10
OCTACOSANE	0.40-0.85	4.9	9
NONACOSANE	0.40-0.85	5.6	10
NONANE, 3-METHYL-	0.31-0.90	1.5	11
NONANE, 2-METHYL-	0.33-0.90	2.8	11
NONANE, 4-METHYL-	0.29-0.89	5.6	11
NONANE, 5-METHYL	0.30-0.89	2.2	11
NONANE, 2,2,4,4,6,8,8-HEPTAMETHYL-	0.24-0.90	21.4	13
OCTANE, 2-METHYL-	0.47-0.57	0.6	9

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
OCTANE, 3-METHYL-	0.46-0.57	0.7	9
OCTANE, 4-METHYL-	0.47-0.57	0.5	9
3-ETHYLHEPTANE	0.46-0.57	0.6	8
HEPTANE, 2,2-DIMETHYL-	0.28-0.90	1.2	25
UNDECANE, 3-METHYL-	0.33-0.90	2.6	11
CYCLOPROPANE	0.37-0.89	2.9	11
CYCLOBUTANE	0.40-0.90	5.5	17
CYCLOPENTANE	0.50-0.63	2.9	15
CYCLOPENTANE, METHYL-	0.48-0.66	0.9	24
CYCLOPENTANE, ETHYL-	0.45-0.66	0.7	21
CYCLOPENTANE, 1,1-DIMETHYL-	0.46-0.68	0.8	15
CYCLOPENTANE, 1,2-DIMETHYL-, cis-	0.39-0.88	1.0	14
CYCLOPENTANE, 1,2-DIMETHYL-, trans-	0.28-0.90	5.9	14
CYCLOPENTANE, 1,3-DIMETHYL-, cis-	0.25-0.89	7.3	11
CYCLOPENTANE, 1,3-DIMETHYL-, trans-	0.25-0.89	4.5	11
CYCLOPENTANE, PROPYL-	0.43-0.63	0.7	21
CYCLOPENTANE,(1-METHYLETHYL)-	0.43-0.63	0.3	14
CYCLOPENTANE, 1-ETHYL-1-METHYL-	0.22-0.89	3.0	14
CYCLOPENTANE, 1-BUTYL-	0.41-0.60	0.6	21
CYCLOHEXANE	0.49-0.66	0.3	20
CYCLOHEXANE, METHYL-	0.44-0.62	1.7	16
CYCLOHEXANE, ETHYL-	0.42-0.58	1.1	15
CYCLOHEXANE, 1,1-DIMETHYL-	0.46-0.56	0.2	15
CYCLOHEXANE, 1,2-DIMETHYL-, cis-	0.45-0.55	0.8	15
CYCLOHEXANE, 1,2-DIMETHYL-, trans-	0.46-0.56	0.2	15
CYCLOHEXANE, 1,3-DIMETHYL-, cis-	0.46-0.56	0.5	15
CYCLOHEXANE, 1,3-DIMETHYL-, trans-	0.46-0.56	0.3	15
CYCLOHEXANE, 1,4-DIMETHYL-, cis-	0.46-0.56	0.2	15
CYCLOHEXANE, 1,4-DIMETHYL-, trans-	0.47-0.57	0.8	15
CYCLOHEXANE, 1,3,5-TRIMETHYL-, trans	0.31-0.84	1.7	11
CYCLOHEXANE, PROPYL-	0.41-0.54	0.5	10
CYCLOHEXANE, (1-METHYL ETHYL)-	0.42-0.53	1.0	19
CYCLOHEXANE,-1,2,3,4-TETRAMETHYL-	0.31-0.90	2.4	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
CYCLOHEXANE, BUTYL-	0.40-0.51	0.9	10
cis-DECALIN	0.35-0.64	3.1	43
trans-DECALIN	0.35-0.66	2.4	44
1,1'-BICYCLOHEXYL	0.40-0.50	0.4	14
CYCLOHEXANE, 1,1-DIETHYL-	0.27-0.90	3.0	11
CYCLOHEXANE, DECYL-	0.35-0.50	1.5	27
CYCLOHEPTANE	0.44-0.65	1.2	19
CYCLOOCTANE	0.44-0.58	1.6	11
CYCLOHEXANE, trans-1,4-DIETHYL	0.31-0.90	2.6	20
HEPTANE, 2,6-DIMETHYL-	0.47-0.64	0.4	25
3-ETHYLPENTANE, 2-2-DIMETHYL-	0.46-0.57	0.5	15
3-ETHYLPENTANE, 2,4-DIMETHYL-	0.46-0.56	0.3	15
ETHENE	0.40-0.68	4.9	21
1-PROPENE	0.53-0.69	0.8	12
1-TRIACONTENE	0.39-0.90	22.3	15
1-BUTENE	0.48-0.79	1.0	16
2-BUTENE, (Z)-	0.31-0.88	3.1	16
2-BUTENE, (E)-	0.59-0.68	7.3	5
1-PROPENE, 2-METHYL-	0.53-0.70	1.8	15
1-PENTENE	0.52-0.64	0.9	6
2-PENTENE, (Z)-	0.60-0.64	0.3	4
2-PENTENE, (E)-	0.60-0.64	0.9	4
1-BUTENE, 2-METHYL-	0.29-0.89	2.8	16
1-BUTENE, 3-METHYL-	0.52-0.66	0.4	9
2-BUTENE, 2-METHYL-	0.43-0.75	1.0	33
1-HEXENE	0.56-0.66	0.5	7
2-HEXENE, (Z)-	0.26-0.88	5.5	11
2-HEXENE, (E)-	0.27-0.90	5.0	11
3-HEXENE, (Z)-	0.27-0.90	4.5	11
3-HEXENE, (E)-	0.31-0.88	5.9	11
1-PENTENE, 2-METHYL-	0.27-0.90	3.1	11
1-PENTENE, 3-METHYL	0.24-0.89	2.4	11
1-PENTENE, 4-METHYL-	0.24-0.89	3.5	11
2-PENTENE, 2-METHYL-	0.27-0.89	5.7	11
2-PENTENE, 3-METHYL-,(Z)-	0.27-0.89	3.5	11
1-HEXENE, 4-METHYL-	0.25-0.88	2.4	11
2-PENTENE, 4-METHYL-, (Z)-	0.28-0.90	3.7	10
2-PENTENE, 4-METHYL-, (E)-	0.26-0.90	3.7	10
PENTANE, 3-METHYLENE-	0.28-0.88	4.7	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1-BUTENE, 2,3-DIMETHYL-	0.23-0.89	5.3	11
1-BUTENE, 3,3-DIMETHYL-	0.33-0.90	2.4	12
2-BUTENE, 2,3-DIMETHYL-	0.38-0.90	0.7	12
1-PENTENE, 2-ETHYL-	0.31-0.90	4.8	11
1-HEPTENE	0.53-0.66	0.1	9
2-HEPTENE, (Z)-	0.26-0.89	5.9	11
2-HEPTENE, (E)-	0.30-0.89	3.0	11
3-HEPTENE, (E)-	0.25-0.88	3.3	11
1-HEXENE, 2-METHYL-	0.32-0.89	3.6	11
1-PENTENE, 3-ETHYL-	0.28-0.90	4.2	11
1-HEXENE, 3-METHYL-	0.28-0.90	1.2	11
1-HEXENE, 3-ETHYL-	0.31-0.69	1.3	20
1-HEPTENE, 4-METHYL-	0.30-0.69	1.5	20
1-BUTENE, 2,3,3-TRIMETHYL-	0.31-0.89	4.4	11
3-HEPTENE, (Z)-	0.25-0.89	5.4	11
1-OCTENE	0.50-0.66	0.3	11
2-OCTENE, (E)-	0.32-0.89	4.1	11
1-PENTENE, 2,4,4-TRIMETHYL-	0.33-0.89	1.4	11
2-PENTENE, 2,4,4-TRIMETHYL-	0.30-0.90	3.1	14
HEPTANE, 3-METHYLENE-	0.33-0.90	3.2	11
NONENE	0.48-0.63	0.5	11
1-DECENE	0.46-0.61	0.5	23
1-UNDECENE	0.43-0.59	0.6	23
1-DODECENE	0.42-0.57	0.7	18
1-TRIDECENE	0.41-0.55	0.7	12
1-TETRADECENE	0.40-0.54	1.0	27
1-PENTADECENE	0.39-0.53	0.7	16
1-HEXADECENE	0.39-0.52	0.9	27
1-OCTADECENE	0.39-0.50	1.4	11
HEPTENE, 6-METHYL-	0.32-0.90	1.2	14
CYCLOPENTENE	0.27-0.90	3.3	30
CYCLOHEXENE	0.43-0.62	0.9	39
trans-2-EICOSENE	0.38-0.90	6.7	15
trans-2-PENTADECENE	0.40-0.89	4.1	19
CYCLOHEPTENE	0.48-0.56	1.1	4
CYCLOOCTENE	0.34-0.90	1.1	12
2-OCTENE, (Z)	0.30-0.90	7.5	10
3-OCTENE, (E)-	0.28-0.89	4.5	11
4-OCTENE, (Z)-	0.27-0.90	1.3	10
4-OCTENE, (E)-	0.31-0.89	3.8	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
3-OCTENE, (Z)-	0.26-0.90	1.8	10
1-HEPTADECENE	0.40-0.51	0.9	20
1-NONADECENE	0.39-0.49	1.2	18
1-EICOSENE	0.39-0.48	1.3	9
CYCLOHEXENE, 4-ETHENYL-	0.27-0.77	2.3	9
CYCLOPENTENE, 1-METHYL-	0.27-0.90	2.7	17
CYCLOPENTENE, 3-METHYL-	0.22-0.90	1.2	13
CYCLOPENTENE, 4-METHYL-	0.21-0.90	6.2	13
HEXENE, 2,3-DIMETHYL-	0.31-0.90	1.2	14
CYCLOHEXENE, 1-METHYL-4-(1-METHYLETHENYL)-, (R)-	0.43-0.65	1.0	21
CYCLOHEXENE, 1-METHYL-4-(1-METHYLETHYLIDENE)-	0.30-0.90	6.0	11
CYCLOHEXENE,1-(2-PROPENYL)	0.31-0.90	1.1	11
1,2-BUTADIENE	0.30-0.99	49.9	22
1,3-BUTADIENE	0.39-0.97	5.1	24
1,2-PENTADIENE	0.27-0.89	6.6	11
1,3-PENTADIENE, (Z)-	0.27-0.89	8.0	11
1,3-PENTADIENE, (E)-	0.37-0.89	6.2	11
1,4-PENTADIENE	0.26-0.89	35.0	14
2,3-PENTADIENE	0.30-0.88	4.8	11
ISOPRENE	0.26-0.88	5.8	11
1,5-HEXADIENE	0.26-0.89	0.7	16
1,2-BUTADIENE, 3-METHYL	0.33-0.90	10.3	11
1,3-CYCLOPENTADIENE, METHYL-	0.28-0.89	2.4	11
1,4-HEXADIENE	0.26-0.90	5.2	13
2,4-HEXADIENE, (E,E)-	0.43-0.89	0.5	11
1,3-CYCLOPENTADIENE	0.37-0.88	11.6	14
4,7-METHANO-1H-INDENE, 3a,4,7,7a-TETRAHYDRO-	0.46-0.89	31.9	11
1,3-CYCLOHEXADIENE, 2-METHYL-5-(1-METHYLETHYL)-	0.34-0.89	11.4	11
CYCLOHEXENE, 3-METHYLENE-6-(1-METHYLETHYL)-	0.34-0.90	7.0	11
1,3-BUTADIENE, 2,3-DIMETHYL-	0.38-0.89	1.7	11
2,4-HEXADIENE, (E,Z)-	0.33-0.89	4.1	11
3-METHYL-1,4-PENTADIENE	0.27-0.90	3.1	18
1,5,9-CYCLODODECATRIENE,(E,E,Z)	0.34-0.90	2.3	11
1,5-HEXADIENE, 2,5-DIMETHYL-	0.35-0.90	3.0	10
2,4-HEXADIENE, 2,5-DIMETHYL-	0.48-0.90	5.1	10
1,3-CYCLOHEXADIENE	0.29-0.90	12.2	14

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1,4-CYCLOHEXADIENE	0.39-0.90	5.2	10
1,5-CYCLOOCTADIENE	0.32-0.89	16.9	12
(3E)-1,3-HEXADIENE	0.40-0.90	1.7	15
(3E)-1,3-PENTADIENE, 2-METHYL-	0.40-0.90	2.2	15
ETHYNE	0.59-0.95	2.7	11
1-PROPYNE	0.58-0.93	4.9	12
1-BUTYNE	0.55-0.85	7.0	20
2-BUTYNE	0.51-1.03	13.2	20
1-PENTYNE	0.35-0.89	30.0	17
3-HEXYNE	0.31-0.88	4.8	11
2-HEXYNE	0.34-0.90	5.5	11
2-PENTYNE	0.32-0.90	14.1	13
1-HEXYNE	0.27-0.89	1.0	12
1-BUTEN-3-YNE, 2-METHYL-	0.33-0.90	7.6	11
1-OCTYNE	0.34-0.90	2.4	22
1-BUTEN-3-YNE	0.40-0.88	4.3	11
1-BUTYNE, 3-METHYL-	0.40-0.89	7.4	11
1-PENTEN-3-YNE	0.29-0.89	4.3	11
1-PENTEN-4-YNE	0.30-0.90	4.5	11
BENZENE, 1,1'-(1,2-ETHYNEDIYL)BIS-	0.40-0.89	0.8	11
1-NONYNE	0.37-0.90	2.5	15
1-DECYNE	0.37-0.90	2.2	15
BENZENE	0.49-0.65	3.4	26
BENZENE, METHYL-	0.46-0.63	0.6	32
BENZENE, ETHYL-	0.44-0.61	1.2	29
BENZENE, 1,2-DIMETHYL-	0.43-0.59	0.4	33
BENZENE, 1,3-DIMETHYL-	0.44-0.61	0.8	22
BENZENE, 1,4-DIMETHYL-	0.44-0.61	0.7	21
BENZENE, PROPYL-	0.43-0.59	0.5	20
BENZENE, 1-METHYLETHYL-	0.43-0.59	0.8	31
BENZENE, 1-ETHYL-2-METHYL-	0.42-0.57	0.5	23
BENZENE, 1-ETHYL-3-METHYL-	0.43-0.59	1.4	26
BENZENE, 1-ETHYL-4-METHYL-	0.43-0.58	1.4	23
BENZENE, 1,2,3-TRIMETHYL-	0.41-0.56	4.2	24
BENZENE, 1,2,4-TRIMETHYL-	0.42-0.58	0.2	27
BENZENE, 1,3,5-TRIMETHYL-	0.40-0.68	1.4	38
BENZENE, BUTYL-	0.41-0.57	0.8	20
BENZENE, (2-METHYLPROPYL)-	0.42-0.57	0.4	16
BENZENE, (1-METHYLPROPYL)-	0.41-0.56	0.8	29

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, (1,1-DIMETHYLETHYL)-	0.41-0.57	0.8	27
BENZENE, 1-METHYL-2-(1-METHYLETHYL)-	0.31-0.90	3.3	14
BENZENE, 1-METHYL-3-(1-METHYLETHYL)-	0.32-0.91	2.2	14
BENZENE, 1-METHYL-4-(1-METHYLETHYL)-	0.32-0.90	6.1	33
BENZENE, 1,2-DIETHYL-	0.41-0.56	0.8	13
BENZENE, 1,3-DIETHYL-	0.41-0.56	1.5	15
BENZENE, 1,4-DIETHYL-	0.42-0.57	1.1	13
BENZENE, 1,2,3,4-TETRAMETHYL-	0.39-0.90	1.4	13
BENZENE, 1,2,3,5-TETRAMETHYL-	0.37-0.90	1.9	14
BENZENE,-1,2,4,5-TETRAMETHYL-	0.52-0.90	3.7	13
BENZENE, 1-tert-BUTYL-4-ETHYL	0.34-0.90	2.1	10
BENZENE, 1,4-BIS(1,1-DIMETHYLETHYL)-	0.50-0.90	1.8	11
BENZENE, PENTAMETHYL-	0.41-0.90	1.1	14
BENZENE, 1,3-bis(1-METHYLETHYL)-	0.31-0.89	36.7	14
BENZENE, 1,4-bis(1-METHYLETHYL)-	0.37-0.89	0.8	14
BENZENE, 1,2,4-TRIETHYL-	0.29-0.84	3.2	10
BENZENE, HEXAMETHYL-	0.58-0.90	6.7	11
BENZENE, 1,2,3-TRIETHYL-	0.32-0.90	5.4	12
BENZENE, HEPTYL-	0.38-0.52	1.3	17
BENZENE, 1,2,3,5-TETRAETHYL	0.36-0.90	1.6	11
BENZENE, DECYL-	0.36-0.50	1.3	35
BENZENE, PENTAETHYL	0.28-0.90	2.6	11
BENZENE, HEXAETHYL-	0.54-0.90	1.9	11
BENZENE, CYCLOHEXYL-	0.38-0.90	10.3	11
BIPHENYL	0.46-0.94	2.8	23
1,1':4', 1"-TERPHENYL	0.55-0.80	3.2	20
1,1':3', 1"-TERPHENYL	0.41-0.82	2.4	31
1,1':2', 1"-TERPHENYL	0.40-0.84	3.3	29
BENZENE, 1,1'-ETHYLIDENEBIS-	0.33-0.90	6.3	13
BENZENE, 1,1'-METHYLENEBIS-	0.39-0.91	2.4	25
BENZENE, (PHENYLETHYL)-	0.42-0.89	4.6	13
BENZENE, 1,1',1"-METHYLIDYNETRIS-	0.42-0.90	4.1	19
BENZENE, PENTYL-	0.40-0.55	0.7	36
BENZENE, HEXYL-	0.30-0.83	4.7	26
BENZENE, OCTYL-	0.38-0.51	1.3	16
BENZENE, NONYL-	0.37-0.50	0.8	13

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, UNDECYL-	0.35-0.90	5.8	11
BENZENE, TRIDECYL-	0.36-0.84	8.7	13
BENZENE, TETRADECYL-	0.36-0.84	9.5	13
BENZENE, DODECYL-	0.35-0.84	7.8	10
1-ETHYL-3,5-DIMETHYL BENZENE	0.29-0.90	4.9	14
2-ETHYL-1,3-DIMETHYL BENZENE	0.38-0.89	3.6	14
BENZENE, 2-ETHYL-1,4-DIMETHYL-	0.33-0.89	4.5	14
BENZENE, 1-ETHYL-,2,4-DIMETHYL-	0.32-0.89	5.2	14
4-ETHYL-1,2-DIMETHYLBENZENE	0.31-0.89	3.8	14
BENZENE, 1-ETHYL-2,3-DIMETHYL-	0.33-0.89	6.4	14
BENZENE, 1,1'-(1,1,2,2-TETRAMETHYL-1,2-ETHANEDIYL)bis-	0.49-0.90	2.2	11
BENZENE, (1-METHYLENEPROPYL)-	0.38-0.89	2.9	11
BENZENE, (1-METHYL-1-PROPENYL)-,(E)-	0.36-0.89	3.6	11
BENZENE, (1-METHYL-1-PROPENYL)-, (Z)	0.42-0.89	1.3	11
BENZENE, 1-METHYL-2-PROPYL-	0.32-0.90	4.1	13
BENZENE, 1-METHYL-3-PROPYL-	0.29-0.90	10.6	13
BENZENE, 1-METHYL-4-PROPYLBENZENE	0.32-0.90	14.3	13
BENZENE,1,1',1''-(1-ETHANYL-2-YLIDENE)tris-	0.39-0.84	3.0	9
BENZENE, 1,1',1'',1'''-METHANETETRAYLTETRAKIS-	0.57-0.90	2.8	10
BENZENE, 1,1',1'',1'''-(1,2-ETHANEDIYLIDENE)TETRAKIS-	0.59-0.90	3.0	10
BENZENE, 1-ETHYL-4-(2 PHENYLETHYL)-	0.38-0.90	3.5	11
BENZENE, 1,2-DIMETHYL-3-PROPYL-	0.36-0.70	4.3	23
BENZENE, 1,2,3-TRIMETHYL-4-ETHYL-	0.37-0.78	1.7	10
BENZENE, 1,2,4-TRIMETHYL-3-ETHYL-	0.37-0.78	1.3	10
BENZENE, 1,2,4-TRIMETHYL-5-ETHYL-	0.38-0.78	1.8	10
1,1'-(1,2-ETHANEDIYL)BIS(4-ETHYL-) BENZENE	0.44-0.80	2.3	10
BENZENE, ETHENYL-	0.43-0.65	14.0	9
BENZENE, 1-ETHENYL-2-METHYL-	0.31-0.89	5.9	14
BENZENE, 1-ETHENYL-3-METHYL-	0.28-0.89	4.8	14

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, 1-ETHENYL-2-ETHYL-	0.30-0.90	5.5	15
BENZENE, 1-ETHENYL-3-ETHYL-	0.26-0.90	7.2	18
BENZENE, 1-ETHENYL-4-ETHYL-	0.33-0.90	7.1	18
BENZENE, 1-ETHENYL-4-METHYL-	0.36-0.89	26.4	11
BENZENE, (1-METHYLETHENYL)-	0.38-0.89	6.8	13
BENZENE, 1,3-DIETHENYL-	0.30-0.89	6.4	11
BENZENE, ETHYNYL-	0.35-0.90	9.8	11
BENZENE, 1-ETHENYL-4-(2-METHYLPROPYL)	0.34-0.90	4.4	11
BENZENE, 1-PROPENYL-,(Z)-	0.32-0.90	12.6	10
BENZENE, 1-PROPENYL-,(E)-	0.36-0.90	7.9	10
BENZENE, 1-ETHENYL-4-(1-METHYLETHENYL)-	0.28-0.83	6.2	9
BENZENE, 1-(1,1-DIMETHYLETHYL)-4-ETHENYL-	0.33-0.90	2.9	10
NAPHTHALENE	0.49-0.66	2.1	21
NAPHTHALENE, 1-METHYL-	0.31-0.90	2.3	34
NAPHTHALENE, 2-METHYL-	0.40-0.89	1.4	19
NAPHTHALENE, 1-ETHYL-	0.35-0.48	1.7	13
NAPHTHALENE, 1,2,3,4-TETRAHYDRO-	0.38-0.52	0.6	18
NAPHTHALENE, 2,6-DIMETHYL-	0.38-0.89	10.1	14
NAPHTHALENE, 1-PHENYL-	0.38-0.89	3.6	11
NAPHTHALENE, 1-NONYL-	0.34-0.89	11.3	11
NAPHTHALENE, 1-DECYL-	0.34-0.89	13.3	14
NAPHTHALENE, 1-BUTYL-	0.35-0.47	1.2	17
NAPHTHALENE, 1-HEXYL-	0.34-0.46	1.5	12
NAPHTHALENE, 2,7-DIMETHYL-	0.38-0.90	11.6	14
NAPHTHALENE, 1-HEXYL-1,2,3,4-TETRAHYDRO-	0.26-0.90	8.1	11
FLUORANTHENE	0.42-0.90	4.1	11
NAPHTHALENE, 1-PROPYL-	0.35-0.48	0.3	15
NAPHTHALENE, 2-ETHYL	0.35-0.48	0.8	18
1H-INDENE, 1-METHYL-	0.40-0.90	1.9	11
1H-INDENE, 2-METHYL-	0.39-0.90	2.2	11
1H-INDENE, 1,2,3-TRIMETHYL-	0.48-0.89	1.9	11
INDENE, 1-PHENYL-	0.40-0.89	2.8	10
BENZENE, 1,1',1"-(1-ETHENYL-2-YLIDENE)TRIS-	0.38-0.89	2.2	11
BENZENE, 1,1',1",1'"-(1,2-ETHENEDIYLIDENE)TETRAKIS-	0.50-0.90	4.9	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
BENZENE, 1,1'-(1,2-ETHENEDIYL)BIS-, (Z)-	0.35-0.90	1.5	10
BENZENE, 1,1'-(1,2-ETHENEDIYL)BIS-, (E)-	0.49-0.90	0.8	10
BENZENE, 1,3-DIMETHOXY-5-(2-PHENYLETHENYL)-,(E)-	0.37-0.90	11.0	15
9H-FLUORENE	0.47-0.90	4.3	10
1H-INDENE	0.40-0.90	59.0	26
ANTHRACENE	0.56-0.90	5.8	12
PHENANTHRENE	0.43-0.89	6.8	13
CHRYSENE	0.54-0.89	2.6	11
PYRENE	0.45-0.89	4.7	11
ACENAPHTHYLENE, 1,2-DIHYDRO-	0.46-0.64	0.5	16
ACENAPHTHALENE	0.46-0.90	1.3	11
TRICYLCO(3.3.1.13,7)DECANE	0.77-0.90	1.9	10
BICYCLO(2.2.1)HEPT-2-ENE, 5-ETHENYL-	0.37-0.84	36.1	9
3,5,1,7-(1,2,3,4)BUTANETETRAYLNAPHTHALENE, DECAHYDRO-	0.66-0.90	3.3	11
1,3-DIMETHYLTRICYCLO[3.3.1.1(3,7)]DECANE	0.35-0.90	2.6	20
BICYCLO(2,2,1)HEPT-2-ENE,2-METHYL	0.37-0.90	3.2	11
BICYLCO(2,2,1)HEPT-2-ENE)5-ETHYL-	0.32-0.90	3.7	11
1H-INDENE, 2,3-DIHYDRO-	0.32-0.98	25.3	39
1,3-CYCLOHEXADIENE, 1-METHYL-4-(1-METHYLETHYL)-	0.34-0.89	3.7	11
1,4-CYCLOHEXADIENE, 1-METHYL-4-(1-METHYLETHYL)-	0.33-0.89	9.2	11
BICYCLO(2.2.1)HEPT-2-ENE	0.55-0.89	1.3	11
BICYCLO(2,2,1)HEPT-2-ENE, 5-ETHYLIDENE-	0.31-0.90	3.6	11
BENZ(a)ANTHRACENE	0.44-0.90	9.4	11
NAPHTHACENE	0.64-0.90	4.0	11
7-ETHENYL-1,2,3,4,4a,4b,5,6,7,9,10-10a-DODECAHYDRO-1,4a,7-TRIMETHYL-1-PHENANTHRENECARBOXYLIC ACID	0.61-0.90	2.6	20

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
[1R-(1 alpha,4 abeta,4 balpha,7 alpha,10 aalpha)]-7ETHENYL-1,2,3,4,4a,4b,5,6,7,8,10,10a-DODECAHYDRO-1,4a,7-TRIMETHYL-1-PHENANTHRENECARBOXYLIC ACID	0.54-0.90	4.4	20
BICYCLO(2.2.1)HEPTANE, 2,2-DIMETHYL-3-METHYLENE-	0.50-0.90	2.1	14
BICYCLO(3.1.1)HEPT-2-ENE, 2,6,6-TRIMETHYL-	0.44-0.64	2.3	40
BICYCLO(3.1.1)HEPTANE, 6,6-DIMETHYL-2-METHYLENE	0.44-0.66	1.2	11
NITROUS OXIDE (N2O)	0.56-0.95	3.3	18
NITROGEN DIOXIDE (NO2)	0.61-0.89	3.0	13
OXYGEN	0.45-0.58	0.6	7
HYDROGEN	0.42-0.96	10.5	28
NITROGEN	0.56-0.71	0.5	6
CARBON MONOXIDE	0.61-0.69	1.5	6
CARBON DIOXIDE	0.73-1.00	18.5	25
SULFUR DIOXIDE	0.52-0.75	3.3	17
SULFUR TRIOXIDE	0.60-0.96	3.1	13
NITROGEN OXIDE (NO)	0.63-0.67	2.7	5
FLUORINE	0.46-0.59	1.7	23
CHLORINE	0.46-0.78	2.3	12
BROMINE	0.48-0.57	0.6	9
OZONE	0.30-0.90	3.3	18
FORMALDEHYDE	0.44-0.89	26.5	11
ACETALDEHYDE	0.32-0.88	19.7	17
PROPANAL	0.38-0.90	19.8	11
3-CYCLOHEXENE-1-CARBOXALDEHYDE	0.27-0.90	8.9	15
BUTANAL	0.33-0.90	14.7	18
PROPANAL, 2-METHYL-	0.41-0.88	14.4	11
PENTANAL	0.32-0.89	15.4	18
HEPTANAL	0.37-0.90	11.3	20
HEXANAL	0.37-0.90	12.0	10
OCTANAL	0.39-0.87	6.2	11
NONANAL	0.39-0.87	15.3	11
HEXANAL, 2-ETHYL-	0.33-0.89	15.2	11
ETHANEDIAL	0.58-0.89	18.6	11
HEXANAL, 2-METHYL-	0.39-0.90	14.8	10

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
HEXANAL, 3-METHYL-	0.39-0.90	13.2	10
2-PENTENAL, 2-METHYL-	0.39-0.90	14.8	11
2-HEXENAL, 2-ETHYL-	0.39-0.90	16.8	11
DECANAL	0.40-0.87	3.9	11
UNDECANAL	0.40-0.82	13.6	10
1-DODECANAL	0.40-0.87	16.9	11
TRIDECANAL	0.40-0.82	16.6	10
BUTANAL, 2-METHYL	0.39-0.90	11.9	16
3-METHYL-BUTANAL	0.41-1.00	18.6	18
2-PROPENAL	0.37-0.88	18.7	20
2-BUTENAL, (Z)-	0.29-1.00	22.2	12
trans-CROTONALDEHYDE	0.35-0.90	16.4	10
2-PROPENAL, 2-METHYL-	0.36-0.90	19.0	11
BENZENEACETALDEHYDE, alpha-METHYL-	0.42-0.90	6.2	16
BENZALDEHYDE, 2-METHYL-	0.34-0.90	14.5	11
BENZALDEHYDE, 4-METHYL-	0.43-0.90	11.8	11
BENZALDEHYDE	0.41-0.54	1.7	23
BENZALDEHYDE, 2-HYDROXY-	0.40-0.68	1.6	15
BENZALDEHYDE, 4-HYDROXY-	0.40-0.55	2.2	15
1,4-BENZENEDICARBOXALDEHYDE	0.53-0.90	15.1	10
BENZALDEHYDE, 3-METHYL-	0.36-0.90	10.7	11
1,3,5-TRIOXANE, 2,4,6-TRIMETHYL-	0.48-0.69	1.5	15
2-PROPANONE	0.54-0.70	2.4	20
2-BUTANONE	0.56-0.60	0.6	6
3-PENTANONE	0.49-0.89	2.3	33
2-PENTANONE, 4-METHYL-	0.34-0.68	7.8	31
2-PENTANONE, 3-METHYL-	0.29-0.89	13.8	21
3-HEPTANONE	0.48-0.60	1.3	21
4-HEPTANONE	0.48-0.60	2.3	23
3-HEXANONE	0.49-0.62	2.0	23
2-PENTANONE	0.51-0.65	1.8	35
2-BUTANONE, 3-METHYL-	0.33-0.90	8.3	21
2-HEXANONE	0.49-0.62	2.0	25
2-HEPTANONE	0.47-0.59	2.0	18
2-HEXANONE, 5-METHYL-	0.33-0.90	15.3	11
3-PENTEN-2-ONE, 4-METHYL-	0.37-0.88	10.6	20
2-BUTANONE, 3,3-DIMETHYL-	0.39-0.89	7.6	21
4-HEPTANONE, 2,6-DIMETHYL-	0.37-0.89	4.9	16
3-PENTANONE, 2,4-DIMETHYL-	0.36-0.90	8.4	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
2-PYRROLIDINONE	0.37-0.90	42.4	11
2-PYRROLIDINONE, 1-METHYL-	0.35-0.90	15.0	17
5-NONANONE	0.45-0.57	1.3	27
2-NONANONE	0.44-0.55	4.8	27
9,10-ANTHRACENEDIONE	0.62-0.90	8.6	11
2,4-PENTANEDIONE	0.44-0.55	2.3	11
2-CYCLOHEXEN-1-ONE, 3,5,5-TRIMETHYL-	0.37-0.89	7.2	13
CYCLOPENTANONE	0.45-0.60	0.9	23
CYCLOHEXANONE	0.43-0.57	3.4	23
2-OCTANONE	0.40-0.90	11.0	26
METHANONE, DIPHENYL-	0.34-0.63	2.5	19
ETHANONE, 1-PHENYL-	0.41-0.64	1.5	17
2-OXETANONE	0.35-0.89	6.0	11
2(3H)-FURANONE, DIHYDRO-	0.31-0.89	3.9	11
2-OXEPANONE	0.35-0.90	2.6	11
2(3H)-FURANONE, DIHYDRO-5-METHYL-	0.33-0.90	12.2	11
2-METHYL, 3-PENTANONE-	0.36-0.90	18.8	21
3-BUTEN-2-ONE, 3-METHYL	0.39-0.88	14.4	11
(1,1'-BICYCLOHEXYL)-2-ONE	0.31-0.90	6.9	11
2,5-CYCLOHEXADIENE-1,4-DIONE	0.58-0.65	0.6	4
2-OXETANONE, 4-METHYLENE-	0.43-0.89	1.7	12
ETHENONE	0.33-0.90	34.0	11
METHANOL	0.53-0.99	5.9	44
ETHANOL	0.53-1.00	4.2	50
1-PROPANOL	0.53-0.68	2.2	17
2-PROPANOL	0.54-0.70	3.5	23
1-BUTANOL	0.49-0.73	2.4	33
1-PROPANOL, 2-METHYL-	0.52-0.68	1.9	15
2-PROPANOL, 2-METHYL-	0.57-0.67	3.5	8
1-PENTANOL	0.46-0.99	19.8	44
2-PENTANOL	0.49-0.88	4.2	38
2-BUTANOL, 2-METHYL-	0.50-0.69	3.4	28
1-BUTANOL, 2-METHYL-	0.34-0.84	8.1	25
1-PROPANOL, 2,2-DIMETHYL-	0.60-0.89	8.4	11
1-HEXANOL	0.45-0.99	9.4	66
2-HEXANOL	0.47-0.71	0.8	27
1-PENTANOL, 2-METHYL-	0.45-0.68	0.3	42
1-PENTANOL, 3-METHYL-	0.47-0.72	2.0	42
3-PENTANOL, 3-METHYL-	0.48-0.67	1.0	43

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
3-PENTANOL	0.37-0.90	9.4	16
1-HEXANOL, 2-ETHYL-	0.32-0.90	13.2	12
1-HEXANOL, 2-METHYL-	0.37-0.90	9.3	11
1-BUTANOL, 3-METHYL-	0.27-0.90	3.9	37
2-BUTANOL, 3-METHYL-	0.34-0.90	11.2	13
1-HEPTANOL	0.43-0.59	1.1	17
2-HEPTANOL	0.45-0.61	0.4	12
1-HEXANOL, 5-METHYL-	0.49-0.90	24.2	11
2-PENTANOL, 4-METHYL-	0.48-0.71	0.3	42
1-OCTANOL	0.42-0.57	2.5	35
2-OCTANOL	0.43-0.59	4.0	21
1-NONANOL	0.41-0.56	0.6	22
2-NONANOL	0.37-0.81	9.9	22
1-DECANOL	0.40-0.54	0.7	22
1-UNDECANOL	0.39-0.53	1.0	13
1-NONANOL, 8-METHYL-	0.33-0.89	12.0	11
1-DODECANOL	0.41-0.52	10.2	35
1-TRIDECANOL	0.40-0.90	9.6	11
1-TETRADECANOL	0.39-0.90	6.4	22
1-PENTADECANOL	0.42-0.90	17.2	10
1-HEXADECANOL	0.39-0.90	4.6	26
1-HEPTADECANOL	0.42-0.90	23.7	10
1-OCTADECANOL	0.38-0.90	5.4	27
1-BUTANOL, 2-ETHYL-	0.27-0.89	7.4	13
1-EICOSANOL	0.42-0.90	25.5	13
1-NONADECANOL	0.42-0.90	22.5	10
CYCLOHEXANOL	0.45-0.57	1.5	12
CYCLOHEXANOL, 1-METHYL-	0.44-0.90	15.5	11
CYCLOHEXANOL, 2-METHYL-, cis-	0.46-0.90	4.7	15
CYCLOHEXANOL, 2-METHYL-, trans-	0.44-0.90	2.6	15
CYCLOHEXANOL, 3-METHYL-, cis-	0.43-0.88	8.2	12
CYCLOHEXANOL, 3-METHYL-, trans-	0.44-0.90	1.6	12
CYCLOHEXANOL, 4-METHYL-, cis-	0.42-0.90	8.9	16
CYCLOHEXANOL, 4-METHYL-, trans-	0.43-0.90	5.8	16
cyclohexanol, 5-methyl-2-1(1-methylethyl)-[1R-{1 alpha, 2-beta, 5 alpha}]	0.48-0.89	1.0	11
STIGMAST-5-EN-3-OL,(3beta)-	0.43-0.90	17.8	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1-NAPHTHALENEMETHANOL, DECAHYDRO-5-(5-HYDROXY-3-METHYL-3-PENTENYL)-1,4a-DIMETHYL-6-METHYLENE-, [1S-[1Alpha,4aAlpha,5Alpha(E),8aBeta]]	0.48-0.96	10.0	14
Alpha,Alpha,4-TRIMETHYL-3-CYCLOHEXENE-1-METHANOL	0.43-0.90	5.9	17
CYCLOHEXANOL, 1-METHYL-4-(1-METHYLETHENYL)	0.44-0.90	4.9	16
1-NONANOL, 2-BUTYL-	0.40-0.90	9.5	15
1-UNDECANOL, 2-METHYL-	0.40-0.90	10.3	16
2-FURANMETHANOL, TETRAHYDRO-	0.46-0.68	1.6	14
2-PROPEN-1-OL	0.50-0.68	1.5	18
BENZENEMETHANOL, alpha,alpha-DIMETHYL-	0.47-0.89	3.5	11
1-OCTANOL, 2-BUTYL	0.29-0.90	12.9	16
PHENOL, 2,3-DIMETHYL-	0.48-0.89	5.5	11
PHENOL, 2,4-DIMETHYL	0.44-0.67	1.1	24
PHENOL, 2,5-DIMETHYL-	0.44-0.67	1.2	19
PHENOL, 2,6-DIMETHYL-	0.43-0.90	5.4	12
PHENOL, 3,4-DIMETHYL-	0.43-0.65	3.4	19
PHENOL, 3,5-DIMETHYL-	0.44-0.66	0.5	19
2-PROPYN-1-OL	0.51-0.57	0.4	4
BENZENEMETHANOL	0.40-0.63	19.7	18
PHENOL	0.39-0.65	1.0	21
PHENOL, 2-METHYL-	0.41-0.76	6.0	26
PHENOL, 3-METHYL-	0.41-0.76	4.3	66
PHENOL, 4-METHYL-	0.42-0.76	7.2	55
PHENOL, 2-ETHYL-	0.38-0.90	21.3	11
1,4-BENZENEDIOL	0.54-0.86	4.7	10
PHENOL, 4-ETHYL-	0.44-0.89	10.3	11
PHENOL, 4-(1,1-DIMETHYLETHYL)-	0.51-0.89	8.0	11
PHENOL, 4,4'-(1-METHYLETHYLIDENE)bis-	0.54-0.89	7.8	10
PHENOL, NONYL-	0.36-0.88	4.7	12
1,2-ETHANEDIOL	0.41-0.57	1.9	11
ETHANOL, 2,2'-OXYBIS-	0.39-0.70	2.3	11
ETHANOL, 2,2'-(1,2-ETHANEDIYLBIS(OXY))BIS-	0.38-0.71	1.9	9
ETHANOL, 2,2'-(OXYBIS(2,1-ETHANEDIYLOXY))BIS-	0.34-0.90	7.2	12

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1,2-PROPANEDIOL	0.34-0.90	7.9	17
1,3-PROPANEDIOL	0.41-0.57	1.4	9
PROPANOL, OXYBIS-	0.36-0.89	13.3	12
1,3-PROPANEDIOL, 2,2-DIMETHYL-	0.64-0.90	11.5	10
2-BUTYNE-1,4-DIOL	0.48-0.90	21.9	10
PROPANOL,((1-METHYL-1,2-ETHANEDIYL)bis(oxy))bis-	0.34-0.90	2.3	11
1,3-PROPANEDIOL, 2-METHYL-	0.26-0.83	32.3	9
1,2-BUTANEDIOL	0.32-0.90	19.2	10
1,3-BUTANEDIOL	0.29-0.90	7.7	15
2,4-PENTANEDIOL, 2-METHYL-	0.36-0.90	2.5	11
1,2,3-PROPANETRIOL	0.35-0.53	2.6	36
1,2,3-BUTANETRIOL	0.38-0.88	15.8	15
1,2,4-BUTANETRIOL	0.39-0.90	31.3	15
1,2-BENZENEDIOL, 4-(1,1-DIMETHYLETHYL-)	0.43-0.90	12.0	10
1,3-PENTANEDIOL, 2,2,4-TRIMETHYL	0.48-0.90	11.8	11
1,3-PENTANEDIOL, 2-METHYL	0.38-0.90	22.6	20
2,3-BUTANEDIOL	0.46-0.89	14.1	11
2-BUTENE-1,4-DIOL, (Z)-	0.42-0.90	21.9	10
2-BUTENE-1,4-DIOL, (E)-	0.45-0.90	22.4	10
1,4-BUTANEDIOL	0.44-0.89	3.7	16
1,5-PENTANEDIOL	0.38-0.89	5.3	12
1,6-HEXANEDIOL	0.43-0.90	12.1	11
1,2-BENZENEDIOL	0.49-0.60	1.2	9
1,3-BENZENEDIOL	0.46-0.56	2.6	7
1,3-PROPANEDIOL, 2,2-BIS(HYDROXYMETHYL)-	0.69-0.89	4.0	11
1,3-PROPANEDIOL, 2-ETHYL-2-(HYDROXYMETHYL)-	0.47-0.89	8.4	12
1,2,3-BENZENETRIOL	0.49-0.90	3.8	10
D-GLUCITOL	0.42-0.89	1.3	11
FORMIC ACID	0.49-0.62	1.0	21
ACETIC ACID	0.49-0.61	2.2	25
PROPANOIC ACID	0.48-0.60	1.7	23
DECANOIC ACID	0.42-0.90	8.5	15
ETHANEDIOIC ACID	0.58-0.90	26.9	11
BUTANOIC ACID	0.47-0.59	2.3	27
BUTANOIC ACID, 2-METHYL-, (+ -)	0.30-0.89	27.0	11
PENTANOIC ACID	0.45-0.57	2.0	23
NONANOIC ACID	0.40-0.90	16.4	16

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
PROPANOIC ACID, 2-METHYL-	0.48-0.67	2.8	26
BUTANOIC ACID, 3-METHYL-	0.46-0.71	5.7	15
HEXANOIC ACID	0.41-0.90	8.9	16
HEXANOIC ACID, 2-METHYL-	0.35-0.90	20.0	15
1,4-CYCLOHEXANEDICARBOXYLIC ACID, trans-	0.66-0.90	17.7	11
OCTANOIC ACID	0.42-0.90	10.5	14
UNDECANOIC ACID	0.41-0.90	18.9	12
CYCLOPENTANEACETIC ACID	0.41-0.90	21.6	11
PROPANOIC ACID, 2,2'-OXYBIS-	0.58-0.90	12.4	11
DODECANOIC ACID	0.43-0.90	5.5	28
TRIDECANOIC ACID	0.42-0.90	10.8	12
TETRADECANOIC ACID	0.43-0.55	2.1	32
HEXADECANOIC ACID	0.43-0.54	1.2	14
2-BUTENOIC ACID, (Z)-	0.45-0.67	9.7	6
2-BUTENOIC ACID, (E)-	0.52-0.89	41.9	11
OCTANOIC ACID, 2-METHYL	0.35-0.95	18.2	14
OCTADECANOIC ACID	0.43-0.85	6.5	15
2-PROPENOIC ACID	0.45-0.89	12.2	23
2-PROPENOIC ACID, 2-METHYL-	0.44-0.90	29.4	11
9-OCTADECENOIC ACID(Z)-	0.38-0.58	0.5	4
9,12-OCTADECADIENOIC ACID(Z,Z)-	0.35-0.89	2.9	11
BENZOIC ACID	0.53-0.90	13.5	16
BENZOIC ACID, 2-METHYL-	0.55-0.63	2.5	7
BENZOIC ACID, 4-METHYL-	0.59-0.90	18.0	11
BENZOIC ACID, 2-HYDROXY-	0.58-0.90	12.5	11
HEXANEDIOIC ACID	0.53-0.90	14.8	11
2-BUTENEDIOIC ACID (Z)-	0.52-0.90	22.9	11
1,2-BENZENEDICARBOXYLIC ACID	0.58-0.89	14.8	11
1,3-BENZENEDICARBOXYLIC ACID	0.62-0.89	23.0	11
ETHANEPEROXOIC ACID	0.49-0.89	60.5	16
ACETIC ACID, ANHYDRIDE	0.42-0.63	2.4	28
PROPANOIC ACID, ANHYDRIDE	0.37-0.90	4.9	25
BUTANOIC ACID, ANHYDRIDE	0.31-0.89	16.3	14
PHENANTHRENECARBOXYLIC ACID, 1,2,3,4,4a,5,6,9,10,10a-DECAHYDRO-1,4a-DIMETHYL-7-(1-METHYLETHYL)-, [1R-(1Alpha,4aBeta,10aAlpha)]-	0.56-1.00	12.6	20
2,5-FURANDIONE, DIHYDRO-	0.49-0.89	5.2	11
2H-PYRAN-2,6(3H)-DIONE, DIHYDRO-	0.39-0.89	7.0	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
1,3-ISOBENZOFURANDIONE	0.51-0.89	2.7	16
2,5-FURANDIONE	0.45-0.90	12.8	11
5-ISOBENZOFURANCARBOXYLIC ACID, 1,3-DIHYDRO-1,3-DIOXO-	0.49-0.90	3.6	11
FORMIC ACID, METHYL ESTER	0.58-0.77	1.7	14
FORMIC ACID, ETHYL ESTER	0.56-0.62	2.3	13
FORMIC ACID, PROPYL ESTER	0.53-0.64	2.6	9
FORMIC ACID, BUTYL ESTER	0.51-0.67	1.8	12
FORMIC ACID, 2-METHYLPROPYL ESTER	0.51-0.67	2.0	12
FORMIC ACID, PENTYL ESTER	0.49-0.65	1.4	13
FORMIC ACID, OCTYL ESTER	0.36-0.89	2.6	14
FORMIC ACID, NONYL ESTER	0.37-0.90	1.6	10
FORMIC ACID, DECYL ESTER	0.37-0.90	1.7	10
FORMIC ACID, ETHENYL ESTER	0.40-0.91	8.6	17
ACETIC ACID, METHYL ESTER	0.56-0.66	1.5	8
ACETIC ACID, ETHYL ESTER	0.54-0.71	1.3	18
ACETIC ACID, PROPYL ESTER	0.52-0.68	0.4	15
ACETIC ACID, BUTYL ESTER	0.49-0.65	0.4	14
ACETIC ACID, 2-METHYLPROPYL ESTER	0.50-0.68	2.4	24
1-BUTANOL, 3-METHYL-, ACETATE	0.33-0.91	1.3	20
ACETIC ACID, 2-PROPENYL ESTER	0.52-0.60	0.1	7
ACETIC ACID, 1-METHYLETHYL ESTER	0.53-0.66	0.9	15
ACETIC ACID, 1-METHYLPROPYL ESTER	0.51-0.67	9.5	18
ACETIC ACID, ETHENYL ESTER	0.35-0.89	1.1	14
PROPANOIC ACID, METHYL ESTER	0.53-0.65	0.3	10
PROPANOIC ACID, ETHYL ESTER	0.52-0.65	0.4	11
PROPANOIC ACID, PROPYL ESTER	0.50-0.69	0.4	18
PROPANOIC ACID, BUTYL ESTER	0.31-0.90	4.5	24
BUTANOIC ACID, PROPYL ESTER	0.46-0.63	0.2	17
PROPANOIC ACID, ETHENYL ESTER	0.35-0.90	3.2	11
BUTANOIC ACID, METHYL ESTER	0.49-0.92	0.9	26
BUTANOIC ACID, ETHYL ESTER	0.48-0.69	0.5	25
PROPANOIC ACID, 2-METHYL-, PROPYL ESTER	0.47-0.64	0.5	27
2-PROPENOIC ACID, METHYL ESTER	0.37-0.89	4.2	22
ACRYLIC ACID, ETHYL ESTER	0.37-0.89	2.4	22
2-PROPENOIC ACID, PROPYL ESTER	0.36-0.89	1.6	11

Table C2. Surface tension data used for model validation (contd.)

Compound Name	Reduced Temperature Range	%AAD	Data points
NONANOIC ACID, BUTYL ESTER	0.35-0.82	1.9	10
PENTANOIC ACID, BUTYL ESTER	0.29-0.89	3.5	16
BUTANOIC ACID, 3-METHYL-, ETHYL ESTER	0.50-0.69	0.7	10
2-PROPENOIC ACID, 2-METHYL-, METHYL ESTER	0.40-0.89	6.7	12
METHACRYLIC ACID, ETHYL ESTER	0.39-0.89	5.8	11
2-PROPENOIC ACID, 2-METHYL-, PROPYL ESTER	0.37-0.89	2.0	11
1,2-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	0.36-0.84	10.2	11
1,2-BENZENEDICARBOXYLIC ACID, DIISOOCTYL ESTER	0.30-0.85	4.6	11
1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER	0.29-0.90	8.0	15
ACETIC ACID, PENTYL ESTER	0.47-0.62	0.4	23
ACETIC ACID, 2-ETHYLHEXYL ESTER	0.28-0.89	3.0	11
ACETIC ACID, PHENYLMETHYL ESTER	0.32-0.72	8.9	8

Table C.3. Comparison of surface tension predictions for non-polar compounds

Compound name	Reduced Temperature Range	Parachor Method (Gold Hammer)*+ (%AAD)	CST Method (Brock and Bird)* (%AAD)	SVRC-QSPR Model (%AAD)
Ethane	0.39-0.97	3.0	2.4	1.8
Propane	0.52-0.98	5.5	1.5	1.6

* Methods recommended by Reid, Sherwood and Prausnitz (Reid, R.C., J.M. Prausnitz, and B.E. Poling, The Properties of Gases and Liquids. 4 ed. 1987: McGraw Hill.)+ The ρ_{Lb} value used for calculation in the Parachor Method (Gold Hammer)*+ comes from the NIST database

Table C.4. Comparison of surface tension predictions for polar compounds

Compound name	Reduced Temperature Range (%AAD)	Parachor Method (Gold Hammer)* (%AAD)	SVRC-QSPR Model (%AAD)
Methanol	0.54-0.97	15.4	1.0
Ethanol	0.53-0.99	4.4	4.2

References

1. Project 801, Physical and Thermodynamic Property Database. Design Institute for Physical Property Data, 1999.

2. Van der Gulik, P.S., Viscosity of saturated R152a measured with a vibrating wire viscometer. Int. J. Thermo physics, 1995. 16(4): p. 874.

3. Jasper, J.J., The Surface Tension of Pure Liquid Compounds. Journal of Physical and Chemical Reference Data, 1972. 1: p. 841.

4. Okada, M.; Higashi, Y., Experimental surface tensions for HFC-32, HCFC-124, HFC-125, HCFC-141b, HCFC-142b, and HFC-152a, Int. J. Thermophysics, 1995, 16, 3, 791-800.

5. Okada, M.; Higashi, Y., Surface tension correlation of HFC-134a and HCFC-123 in CFCs, The Day After (Proceedings of the Joint Meeting of IIR Commissions B1, B2, E1, and E2), Padua, Italy, International Institute of Refrigeration, Paris, 1994, 541-548.

6. Baidakov, V.G.; Sulla, I.I., Surface tension of propane and isobutane at near-critical temperatures, Russian Journal of Physical Chemistry, 1985, 59, 551-55.

VITA

Ajay Jegadeesan

Candidate for the Degree of

Master of Science

Thesis: STRUCTURE-BASED GENERALIZED MODELS FOR SELECTED PURE-FLUID SATURATION PROPERTIES

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Chennai, India, December 16, 1981, the son of Jegadeesan Subbarayan and Shanthi Jegadeesan.

Education: Graduated from SBOA Matriculation and Higher Secondary School, Chennai, India. Received the Bachelor of Engineering (Honors) degree in Chemical Engineering from Birla Institute of Technology and Science (BITS), Pilani, India, in May 2003. Completed the requirements for Master of Science degree in December 2006.

Experience:
Validation Lead, Tata Consultancy Services, India (Jun 2003 -Jul 2004)
Teaching Assistant, Oklahoma State University, Stillwater (Jan 2005-Dec 2005)
Research Assistant, Oklahoma State University, Stillwater (Aug 2005-Jul 2005)

Professional Memberships:
Student Member, Society of Petroleum Engineers (SPE)
Student Member, Society of Exploration Geophysicists (SEG)
Student Member, American Society for Chemical Engineers (AIChE)
Student Member, American Society for Quality (ASQ)

Name: Ajay Jegadeesan **Date of Degree**: December, 2006

Institution: Oklahoma State University **Location**: Stillwater, Oklahoma

Title of Study: STRUCTURE-BASED GENERALIZED MODELS FOR SELECTED PURE-FLUID SATURATION PROPERTIES

Pages in Study: 115 Candidate for the Degree of Master of Science

Major Field: Chemical Engineering

Scope and Method of Study:

This study focused on developing structure-based predictive models for prediction of pure-fluid surface tensions and saturation viscosities. Reliable experimental data for a wide range of molecular species was assembled from the DIPPR physical property database. The scaled-variable-reduced-coordinate (SVRC) framework was used to correlate the available data for the saturation properties under consideration. Quantitative structure-property relationships (QSPR) modeling was used to generalize the SVRC model parameters. Non-linear QSPR models involving a hybrid of Genetic Algorithms (GA) and Artificial Neural Networks (ANN) were developed for the model parameters.

Findings and Conclusions:

The SVRC-QSPR model, in general, was found to be capable of providing generalized *a priori* predictions for pure-fluid surface tensions and saturation viscosities with an absolute average deviation of 2%, based on end-point input data. The results of this study indicate that the use of theory-framed structure-property modeling is effective in thermo-physical model generalization.

ADVISER'S APPROVAL: Khaled. A.M. Gasem