COMPUTERIZED PREDICTION SYSTEM FOR THERMOPHYSICAL PROPERTIES①

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ABSTRACT The construction in the initial stage of a sulr-system (PHYSDPRE) for prediction of thermophysical properties in Intellectualized Data-base Management System on Kinetics of Metallurgy(IDMSKM) has been proposed. PHYSDPRE possesses a highly modularized structure, an user friendly interface and comparatively complete auxiliary functions. Using a computer optimization method, the density, viscosity as well as surface tension for binary metallic and ionic melts could be evaluated with a reasonable accuracy by PHYSDPRE. Also the transport properties for low density gases and gas mixtures could be adequately predicted. With density and viscosity in binary metallic and ionic melts as examples, guidelines for model predictions are especially emphasized.

Key words prediction of thermophysical property intellectualized data-base management system metallic melt ionic melt

1 INTRODUCTION

Physical property data are essential for mechanism studies, the optimization and on-line control of existing processes, even for new process designs. The earliest integrated computerized thermophysical data-base for metallic materials production processes may be the KINDAS system[1] at RWTH Aachen. CLIPPER and FORTRAN were employed for coding, which may make the system not very convenient to reach a perfect visual display.

The development of Intellectualized Data-base Management System on Kinetics for Metallurgy (IDMSKM)[2] was started in 1994 aiming at establishing a comprehensive and user-friendly data-base system for physical properties with their applications to the kinetics in metallic materials processing.

This paper mainly presents the construction of a sulr-system for the prediction of thermophysical properties, PHYSDPRE.

2 GENERAL DESCRIPTION

It has long been thought that the experimental physical property data available for molten systems are too few to meet the requirements of process simulation and design. On the other hand, many investigators have contributed towards developing mathematical models to evaluate physical property data for some molten phases. This situation promotes and enables us to organize the available models in a software system for physical property estimations.

The hardware configuration for the system required includes an IBM compatible computer with a 486 or higher processor, at least 8 Mbytes Ram and a 340 Mbytes hard disk. The software environment involves the use of MS Windows as a work-bench and FoxPro 2.5 for Windows and MS C/C++ as the programming languages.

The structure of IDMSKM is illustrated in Fig. 1. In addition to the main menu and coordi-

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nator, PHYSDBMS surrounded by the left dashed square in the lower part of this figure is the module for the management of the containing experimental property data stored in one of its components, DDBFS. Detailed information regarding PHYSDBMS has been reported in Ref [2]. In the middle of lower part, PHYSDPRE, the module parallel to PHYSDBMS, is the subsystem for predictions of physical property data. Up to now, PHYSDPRE has been able to evaluate the density, viscosity, surface tension data in unary and binary metallic and ionic melts with a satisfactory accuracy, and to predict transport properties in low density gaseous systems. More concrete presentation is given in the following sections.

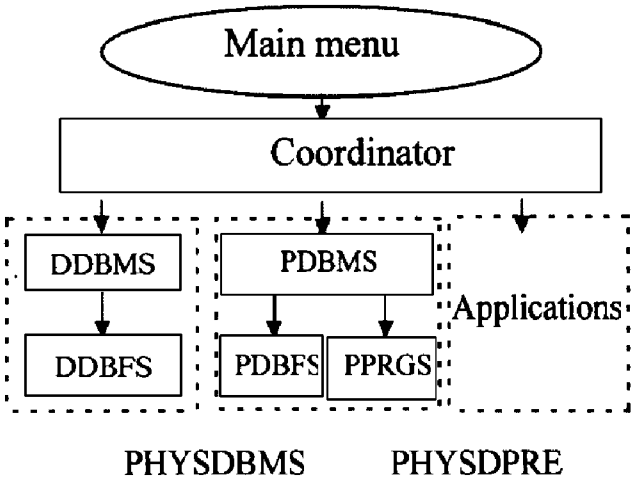

Fig. 1 Module structure of IDMSKM system

3 EVALUATION OF PHYSICAL PROPERTIES

In the construction of PHYSDPRE, the selection as well as the development of suitable models are crucial. The model reliability is of the most importance among the guidelines for model selections. Of course, the model generality and simplicity should also be comprehensively considered.

3.1 Molten systems

Under guidelines mentioned above, primarily semi-theoretical and semi-empirical procedures have been involved for molten systems. In the remaining portion of this section, emphasis will be focused on the considerations of model selection with a few examples, rather than to list the equations involved in the models.

For pure liquid metals, oxides and halides, the relationship of density (ρ) with temperature (T) can be expressed by the following equation:

$$\rho = D_0 + D_1 T + D_2 T \ln T \quad (1)$$

For binary metallic and ionic melts such as oxide or halide mixtures, the empirical relationship of the density with composition (X) and temperature can be presented as

$$\rho = \Sigma D_k X^k \quad (2)$$

$$D_k = D_{0k} + D_{1k} T + D_{2k} T \ln T \quad (3)$$

where X presents mole fraction for one of the components, and T for temperature in k. With k = 0, 1, 2, the optimized results may reach a satisfactory accuracy. As examples Figs. 2 and 3 show a comparison between the model calculated and measured densities in molten Bi-Te[3] and K_2O-B_2O_3[4] systems respectively.

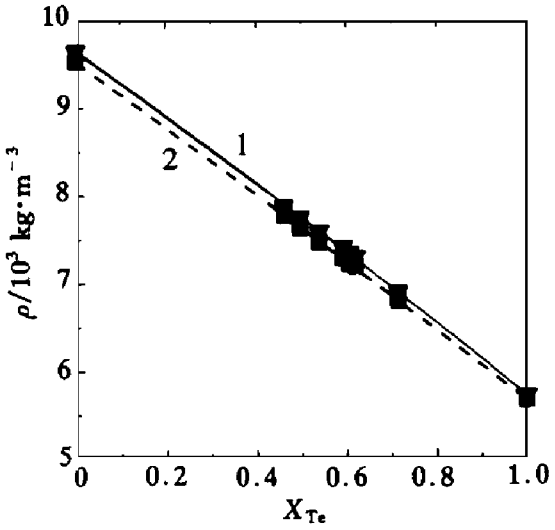

Fig. 2 Comparison between calculated and measured densities in Bi-Te system

1—873 K; 2—973 K

Regarding the evaluation for viscosities in metallic and ionic melts[6, 7], models based on Eyring's absolute reaction rate theory have been employed. The main assumption correlating viscosity η and temperature T in these models can be expressed as

$$\eta = \frac{hN\rho}{M} \exp\left(\frac{\Delta G^{\neq}}{RT}\right) \quad (4)$$

In Eqn. (4), h is Planck's constant, N is Avagadro's number, M and ρ respectively represent the molecular mass and the density in the molten systems, $\Delta G^{\neq}$ denotes the activation energy of viscous flow. For pure liquid system

$$\Delta G^{\neq} = L_0 + L_1 T + L_2 T \ln T \quad (5)$$

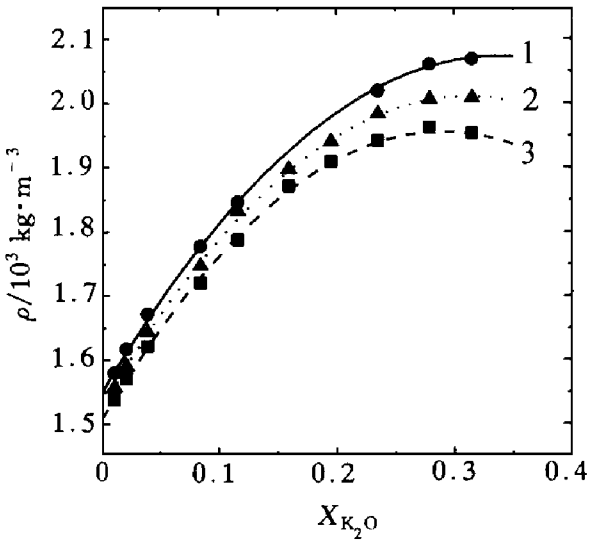

Fig. 3 Comparison between calculated and measured densities in K_2O-B_2O_3 system

1—973 K; 2—1 073 K; 3—1 173 K

For high-order systems, $\Delta G^{\neq}$ has been correlated with mole fraction of each component X_i and temperature T. For binary metallic melts[5, 6], the relationship can be expressed as

$$\Delta G^{\neq} = X_1 \Delta G_1^{\neq} + X_2 \Delta G_2^{\neq} + RT(X_1 \ln X_1 + X_2 \ln X_2) + \Delta^E G^{\neq} \quad (6)$$

The relationship of $\Delta^E G^{\neq}$, which has been named as excess activation energy of viscous flow by the present authors[5], with X_i and T can be written as

$$\Delta^E G^{\neq} = X_1 X_2 \Sigma^k L (X_1 - X_2)^k \quad (7)$$

and

$${}^k L = {}^k L_0 + {}^k L_1 T + {}^k L_2 T \ln T \quad (8)$$

It is noted that the above expressions take a similar form as Margules model and Redlich formulae for the excess Gibbs energy in solution systems. For molten ionic systems, Eqns. (6) ~ (8) have been replaced by equations[6] with similar formalism to the two-sublattice model for the Gibbs molar energy of molten systems with different tendency for ionization[7].

Considering the non-ideal behavior of the high-order molten systems, densities were first optimized by Eqns. (2) and (3) instead of using a linear summation of the densities of all the pure components as in Ref[6]. With the optimized values of ρ, the viscosities were evaluated. This modification would help to attain kinematic viscosity values with a better accuracy, as known, which are very important to process dynamics. Fig. 4 demonstrates a comparison between calculated and measured[3] viscosities in Bi-Te system and Fig. 5 shows the corresponding kinematic values for the same system. For the sake of brevity, examples for the ionic system will not be illustrated in this paper.

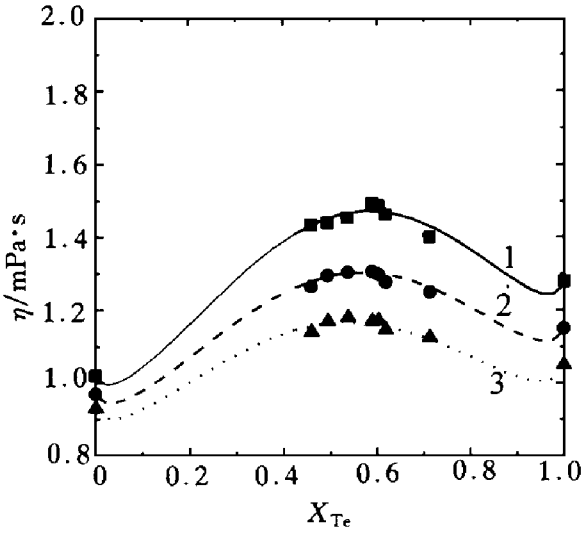

Fig. 4 Comparison between calculated and measured viscosities in Bi-Te system

1—873 K; 2—923 K; 3—973 K

The concept of excess quantities has been applied to other intensive properties, for example the surface tension in present system, which would allow the optimization of those properties readily be carried out. Although the optimization procedure applied in the present study requires a few experimental data as basis, however it may yield a satisfactory accuracy. Moreover, this would enable us to employ the approach analogous to CALPHAD technique for excess Gibbs energy calculations in solution systems, which might make it possible to predict the physical

properties of higher-order systems with the relevant information in the constituent lower-order systems.

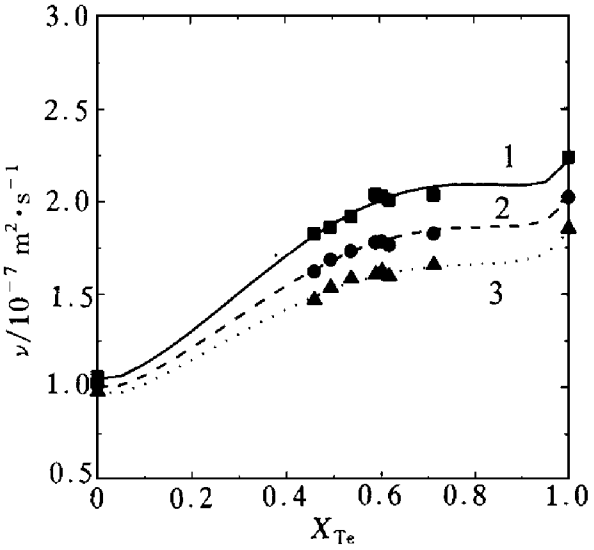

Fig. 5 Comparison between calculated and measured kinematic viscosities in Bi-Te system

1 —873 K; 2 —923 K; 3 —973 K

3.2 Gaseous systems

The predictions for gaseous phases in PHYSDPRE are limited to transport properties, such as viscosity, diffusivity and thermal conductivity in low density gaseous systems. The models for the estimation of those properties are based on Chapman-Enskog's kinetic theory[8] for gases. The viscosity of a pure gas, μ(in Pa·s), can be evaluated by

$$\mu = 2.6693 \times 10^{-8} \frac{(MT)^{1/2}}{\sigma^2 \Omega_\mu} \quad (9)$$

where M is molecular mass of the gas, σ is collision diameter in nm and Ω_μ is collision integral. Ω_μ can be calculated with the help of Lennard-Jones potentials table. The Chapman-Enskog theory can be extended to gas mixtures and the following expressions for the viscosity,

$$\mu_{mix} = \Sigma\left(\frac{X_i \mu_i}{\phi_i}\right) \quad (10)$$

$$\phi_i = \sum_j X_j \phi_{i,j} \quad (11)$$

$$\phi_{i,j} = \frac{[1 + (\frac{\eta_i}{\eta_j})^{1/2}(M_j/M_i)^{1/4}]^2}{[8(1 + M_i/M_j)]^{1/2}} \quad (12)$$

where i, j stand for the pure gas components; M_i, M_j and μ_i, μ_j designate the molecular masses and viscosities for i, j respectively. The relative deviations between calculated and measured values for pure gases have been found to be less than 2% ~ 3%. For the estimation of thermal conductivities in pure gases, the relative deviations between calculated and measured pure gases were found to be less than 5% ~ 7%. As the lack of the experimental data for the transport properties of gas mixtures right now, it may be difficult to make an accurate comparison between model predicted and experimental data. However with the present system, at least, one may have the roughly estimated transport property values for gas mixtures required. More detailed description will be presented elsewhere.

4 DESIGN OF PHYSDPRE PACKAGE

In the design of PHYSDPRE, the source programs of mathematical models for the physical property calculations were mainly written in C language and converted to .fll files using MS C/C++ 7.0 compiler. With the FoxPro external interface L. C. K., .fll files can be linked with FoxPro programs, i. e. the .prg files. In this way, PHYSDPRE may benefit from the advantages of C such as the higher speed, the large amount of functions as well as higher precision.

The structure of PHYSDPRE is illustrated in Fig. 6. The three sub-modules, PDBMS, PDBFS as well as PPRGS with their functions are also respectively described in this figure. Other features of PHYSDPRE such as the user-friendly interface, the flexibility in selecting of the data display or output mode are in common with PHYSDBMS[2].

5 FUTURE WORK

The scope of the system is being expanded in a number of aspects. First, this extension comprises the prediction of the properties in higher order systems. Secondly, the consideration involves the prediction of physical property values with thermodynamic property information. Furthermore, a module APPLICATIONS, parallel to PHYSDBMS and PHYSDPRE, is un-

der nvestigation, which would make it possible to answer users' inquiries of predictions of metallurgical process kinetics. Finally, the development of a module for the assessment of physical properties in molten systems will, as a special issue, be taken into account.

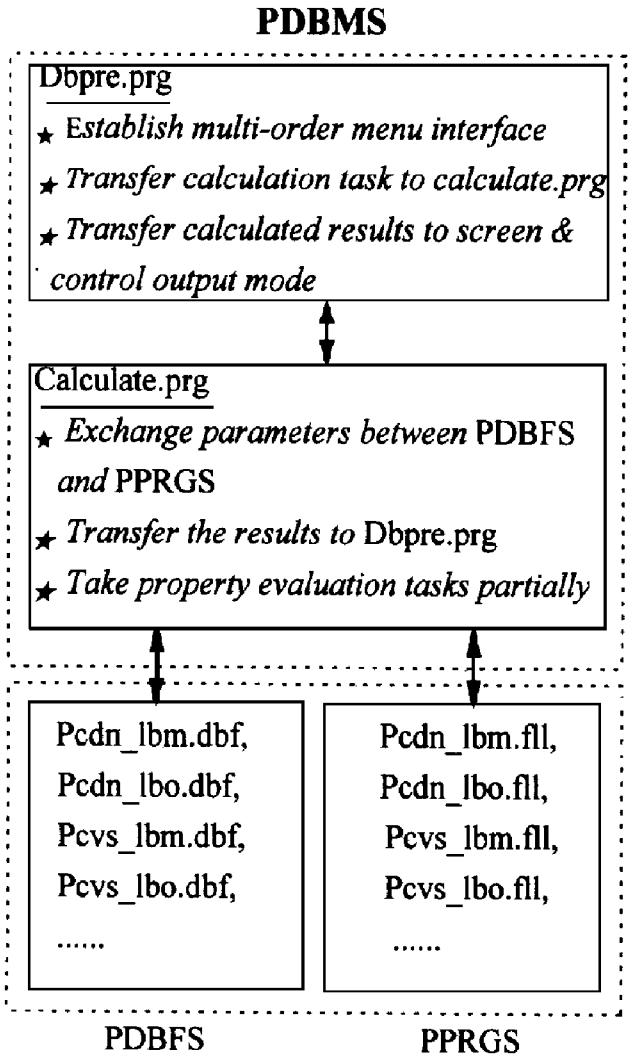

Fig. 6 Structure and function of PHYSDPRE

PDBFS—Package of databases for optimized parameters or coefficients; PPRGS—Program package for property calculation models

6 SUMMARY

(1) The present system, PHYSDPRE in IDMSKM is able to serve users' retrievals of model, predicting data with a satisfactory accuracy for density, viscosity and surface tension in unary and binary metallic or ionic melts. PHYSDPRE is also capable of predicting transport properties of pure gases as well as gas mixtures.

(2) Using FoxPro and C hybrid programming technique, PHYSDPRE takes the advantages from both the systematic softwares, such as high speed, higher precision and the flexibility for characters processing.

(3) The highly modularized structure and the completed auxiliary functions may make it easy for the enhancement of its capabilities of the present system.

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