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Original Study Article

# Thermal energy transfer models in the heat exchange equipment calculations

Alexey A. Kryukov, Leonid A. Marushin, Olga B. Sennikova, Gleb V. Semochkin

Moscow Polytechnic University, Moscow, Russia

ABSTRACT

***BACKGROUND:*** Studies in the field of heat transfer in the heat exchange equipment show significant deviations in calculations when the thermophysical properties of materials are assumed to be averaged. This creates problems in design and reduces the efficiency of heat exchangers.

***OBJECTIVE:*** Building and implementation of the heat transfer models that consider variations in temperature within the thermal properties of materials, with the goal of enhancing the precision of heat transfer predictions and optimizing the design of heat exchange systems.

***METHODS:*** The study utilized numerical analysis of heat transfer considering temperature variations of thermophysical properties. Heat transfer agent mobility and relaxation models were applied. The study included the analysis of density, average flow rate of heat transfer agents, thermal conductivity coefficient, specific heat capacity, relaxation time and free path length. The evaluation methods included mathematical modeling and numerical calculations.

***RESULTS:*** The analysis showed that the use of the models that take into account temperature dependencies significantly improves the accuracy of heat transfer calculations. The heat transfer coefficient, heat transfer agent mobility and relaxation time were found to depend significantly on temperature. Qualitative changes in the mobility of heat transfer agents as a function of temperature and the aggregate state of the material were determined.

***CONCLUSIONS:*** The proposed models of mobility and relaxation of heat transfer agents allow to predict heat transfer more accurately, which improves the design of heat exchangers and increases their efficiency in industry. These models can be used for further research and optimization of heat transfer systems.

**Keywords:** heat transfer; heat exchange equipment; temperature dependence; thermophysical properties; mobility models; heat transfer calculation.

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Оригинальное исследование

# Модели переноса тепловой энергии в расчётах теплообменного оборудования

А.А. Крюков, Л.А. Марюшин, О.Б. Сенникова, Г.В. Сёмочкин

Московский политехнический университет, Москва, Россия

АННОТАЦИЯ

**Обоснование.** Исследования в области теплопереноса в теплообменном оборудовании показывают значительные отклонения в расчётах, когда теплофизические свойства материалов принимаются усреднёнными. Это создаёт проблемы в проектировании и уменьшает производительность теплообменных аппаратов.

**Целью работы** является разработка и внедрение моделей теплопередачи с учётом температурных изменений тепловых характеристик материалов с целью повышения точности прогнозов теплопередачи и создания оптимальных конструкций теплообменного оборудования.

**Методы.** В исследовании использовался численный анализ теплопереноса с учётом температурных изменений теплофизических свойств. Были применены модели подвижности и релаксации теплоносителей. Исследование охватывало анализ таких параметров, как плотность, средняя скорость движения теплоносителей, коэффициент теплопроводности, специфическая теплоёмкость, время релаксации и длина их свободного пути. Методы оценки включали математическое моделирование и численные расчёты.

**Результаты.** Анализ показал, что использование моделей, учитывающих температурные зависимости, значительно улучшает точность расчётов теплопередачи. Было выявлено, что коэффициент теплопроводности, подвижность носителей и время релаксации существенно зависят от температуры. Определены качественные изменения подвижности тепловых носителей в зависимости от температуры и агрегатного состояния материала.

**Заключение.** Предложенные модели подвижности и релаксации тепловых носителей позволяют более точно прогнозировать теплопередачу, что улучшает проектирование теплообменных аппаратов и повышает их эффективность в промышленности. Эти модели могут быть использованы для дальнейших исследований и оптимизации теплопередающих систем.

**Ключевые слова:** теплоперенос; теплообменное оборудование; температурные зависимости; теплофизические свойства; модели подвижности; расчёт теплопередачи.

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## BACKGROUND

To analyze a heat exchanger or its components based on temperature-related variations in properties, it is reasonable to use appropriate models and dependencies rather than conventional av-erage values. This approach better accounts for the laws of energy transfer and the properties of thermally conductive materials. Numerical studies [1–4] have showed deviations, often significant, as a result of temperature dependence of thermophysical properties on the calculations, where the averaged properties were taken in the operating temperature range.

According to an orthodox theory [1], the conductivity factor is determined by the following formula:

$$\lambda = \frac{1}{3} c \cdot \rho \cdot \overline{v} \cdot \overline{l} \,, \qquad (1)$$

where $c$ is the specific thermal capacity, $\rho$ is the density, and $\overline{v}$ and $\overline{l}$ are the average velocity of heat carriers and their mean free path.

This dependence may also be represented as follows:

$$\lambda = \frac{1}{3} c \cdot \rho \cdot \left(\overline{v}\right)^2 \cdot \overline{\tau} \,, \qquad (2)$$

where $\tau$ is the average carrier relaxation time.

The mobility of a particle which carries energy within materials is known to be expressed by the equation:

$$u = \frac{\overline{v}}{F}, \qquad (3)$$

where $\overline{v}$ is the average speed of the particle, and $F$ is the total force effect during its movement.

According to Nernst–Einstein [3], the mobility during mass transfer may be represented as:

$$u = \frac{D}{k \cdot T} \,, \qquad (4)$$

where $D$ is the diffusion factor, and $k$ is the Boltzmann constant.

When electrons transfer heat, their mobility is expressed by the equation:

$$u = \frac{a}{k \cdot T} \cdot e \,, \qquad (5)$$

where $a$ is the thermal diffusivity equal to $\left(\frac{\lambda}{c \cdot \rho}\right)$, and $e$ is the elementary charge.

Following this approach, the authors propose to express the mobility during heat transfer by phonons as:

$$u = \left(\frac{a}{k \cdot T}\right) \cdot k = \left(\frac{a}{T}\right). \qquad (6)$$

According to contemporary theories, "The mechanisms of carrier dispersion are determined quite accurately by the degree ($x$) in the variation of mobility respective to temperature expressed as $U \approx T^X$. It should be noted that at the moment of heat transfer, carriers often scatter with various objects (electrons, phonons, impurities, etc.); therefore, the value of degree $x$ is a certain average value and it is usually difficult to accurately determine the type of scattering" [4, p. 44].

Considering the relationship between carrier mobility, relaxation time, and the mean free path, thermal conductivity may be analyzed using the relaxation model.

This model can be represented by formula:

$$\lambda = \frac{1}{3} c \cdot \rho \cdot \left(\overline{v}\right)^2 \cdot \tau_p^{n_p} \,. \qquad (7)$$

This expression still implies the problem of choosing the correct average velocity of carriers, especially with a view to its temperature dependence. We should solve it by analyzing carrier dissi-pation mechanisms, the substance structure, and the carrier type. The same issues are inherent in the values of $n_p$.

## TEMPERATURE DEPENDENCE ANALYSIS

Values of this variable in equation (7) determine the probable number of scattering events during the heat transfer process. In case there is no carrier scattering at all, $n_p$ is equal to zero; and at maximum scattering, the relaxation time may be described by the following expression:

$$\overline{\tau}_p = \frac{\hbar / kT}{\exp\left(\frac{T_{\max}}{T}\right) \pm 1}. \qquad (8)$$

Here, $n_p$=1. It indicates that temperature variations of degree n in the range from 0 to 1 reflect the entire complexity and diversity of processes accompanying the dissipation of carriers. These variations can be evaluated by the following reasoning.

As the temperature increases, the average relaxation time decreases, because the increase in temperature leads to increased excitation of particles causing an increased frequency of peaks of all waves and reduced intervals between interactions. In case of complete scattering ($n_p$=1), the contribution of the transported particles, which is proportional to the thermal conductivity, increases as the average relaxation time is reduced. This is due to the fact that, at low temperatures, the probability of wave scattering is insignificant and the number of scattering centers in a substance is limited only by waves associated with electrons, phonons, photons, etc. Under these

conditions, the waves normally do not lose their energy and scatter freely.

An important question that follows from this analysis is how the dependence $n_p = f(T)$ is determined and how these values can be calculated.

We can observe that, in the solid state of the material at low temperatures $(T < \theta_v)$, $n$-value remains marginal, which is explained by the freezing of most monochromatic waves and the limited number of scattering centers in the substance.

However, when the temperature rises to a certain level (defrosting), the processes are activated, which leads to a sharp increase in the value of $n_p$. Further temperature increase leads to a slight increase in the $n$ factor.

In the liquid state, the thermal conductivity for the same values of $n$ is lower than in the solid state and is even lower in the gaseous state. In both cases, temperature variations have a less significant effect on $n_p$. The $n$-value in the liquid state is lower than that in the solid state because there are no long-range ordering or solid-related defects, and the scattering processes are concentrated mainly at short distances, i.e. within the first coordination sphere.

Being save for short-range interactions, in the gaseous state the main source of scattering is molecules, which further reduces the value of $n$ as compared to the liquid state.

Of note, $n$ is a very sensitive parameter. Even minor variations up to the third decimal place can significantly affect the average relaxation time and, accordingly, the thermal conductivity. Therefore, the $n_p = f(T)$ dependence shall consider all possible factors.

If $n$ is taken to be equal to zero (i.e. if there are no scattering processes in the substance), the thermal conductivity at a given temperature reaches its limit. At a temperature characteristic of the solid state, the highest thermal conductivity is achieved, which is determined only by the heat capacity, density, and speed of the carriers. Thus, the proposed model allows to solve the problem of determining the maximum thermal conductivity of real materials, which has not been proven in the literature before.

Obviously, to obtain numerical values of $n_p$, it is first required to determine the average velocity of heat carriers. Unfortunately, there is no exact solution for the values of velocity, mean free path, and relaxation time of heat carriers; therefore, $n_p$ value does not exist in theoretical physics.

Thus, the authors recommend to determine carrier dissipation mechanisms using the mobility model.

In addition to the above-mentioned electrons, phonons, and molecules, heat transfer carriers and scattering sources in some substances, such as semiconductors, amorphous structures and gases, may also include photons, electrons, and other high-energy particles. No doubt, their role will be considered in further analysis of various substances.

However, no above models can be a simple solution to the problem of the applicability of carrier dissipation mechanisms.

The most developed model for heat exchange equipment calculations is the mobility model, where the temperature degree x allows to evaluate the type of electron scattering. There's no such dependence for phonons and additional heat transfer mechanisms.

To date, there are studies of thermal conductivity of powdered silicon dioxide ($SiO_2$), used as an additive in the production of refractory structures, and fused amorphous $SiO_2$. However, we believe that heat transfer in these materials is not yet complete. Temperature dependences of thermal conductivity for fused quartz and quartz glass calculated using the energy carrier mobility model are shown in Fig. 1.

In this case, the movement of electrons is determined by their scattering on thermal lattice vibrations, i.e. phonons, at elevated temperatures ($T$>50÷70 $K$). Proportional dependence of mobility $U$ on temperature $U \sim T^{-1.5}$ is characteristic of this process.

However, it should be considered that additional scattering mechanisms caused by impurities often become as significant as the basic electron-phonon interaction.

## CONCLUSION

Numerical studies have shown that if temperature dependences of thermophysical properties are considered, it significantly increases the accuracy of calculations compared to conventional methods, where the properties of materials are taken as averaged. The proposed model of carrier mobility and relaxation allows for more accurate predictions of heat transfer processes in heat exchangers based on various scattering mechanisms (electrons, phonons, and impurities) and their interaction depending on the temperature and state of the substance. Analysis of temperature dependences of thermal conductivity and relaxation time showed significant variations in material properties relative to temperature variations, which shall be considered to improve the performance of heat exchange equipment. This model allows for more accurate determination of the average carrier velocity and other key parameters. Further research will focus on expanding the model to consider more complex operating conditions and analyzing different types of heat exchangers.

## ADDITIONAL INFORMATION

**Authors' contribution.** A.A. Kryukov — search for publications, writing the text of the manuscript O.B. Sennikova — editing the text of the manuscript;

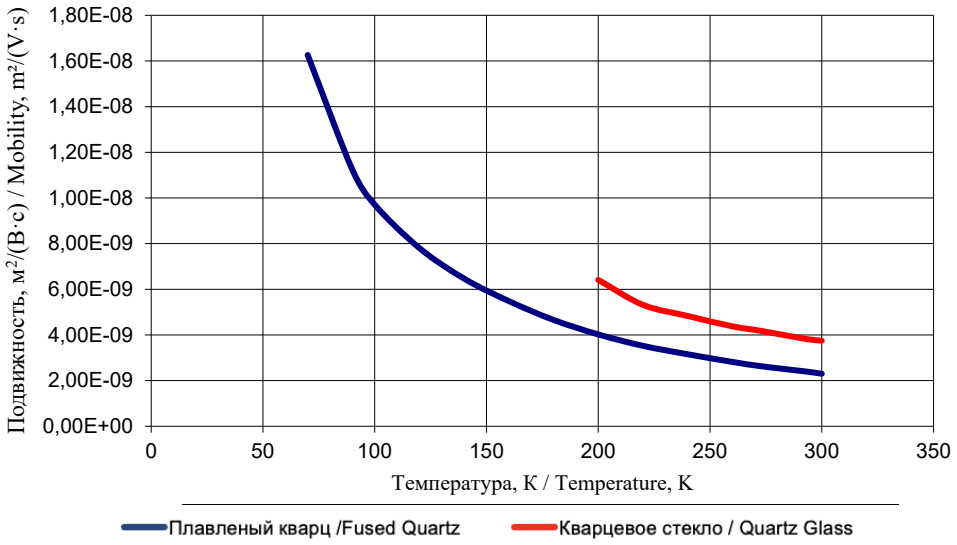


**Fig. 1.** Dependence of silicone dioxide mobility in temperature.
**Рис. 1.** Температурные зависимости подвижности двуокиси кремния.

L.A. Marushin — expert opinion, approval of the final version; G.V. Semochkin — search for publications on the topic of the article. All authors made a substantial contribution to the conception of the work, acquisition, analysis, interpretation of data for the work, drafting and revising the work, final approval of the version to be published and agree to be accountable for all aspects of the work.

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## ДОПОЛНИТЕЛЬНАЯ ИНФОРМАЦИЯ

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## AUTHOR'S INFO

*** Alexey A. Kryukov,**
Student of the Industrial Heat Power Engineering Department;
address: 38 Bolshaya Semenovskaya st, Moscow,
Russia, 107023;
ORCID: 0009-0003-5460-5208;
eLibrary SPIN: 3780-7865;
e-mail: AlexseyKryukov@yandex.ru

**Leonid A. Maryushin,**
Cand. Sci. (Engineering), Associate Professor,
Professor of the Industrial Heat Power Engineering Department;
ORCID: 0009-0000-5240-0186;
eLibrary SPIN: 3812-2917;
e-mail: katzbalger@yandex.ru

**Olga B. Sennikova,**
Cand. Sci. (Engineering), Associate Professor,
Professor of the Industrial Heat Power Engineering Department;
ORCID: 0009-0002-0069-5669;
eLibrary SPIN: 6470-5501;
e-mail: borjusya@yandex.ru

**Gleb V. Semochkin,**
Student of the Management Department;
ORCID: 0009-0000-4269-4678;
eLibrary SPIN: 3228-5831;
e-mail: glebsem03@gmail.com

* Corresponding author / Автор, ответственный за переписку

## ОБ АВТОРАХ

*** Крюков Алексей Алексеевич,**
студент кафедры «Промышленная теплоэнергетика»;
адрес: Россия, 107023, Москва,
ул. Большая Семёновская, д. 38;
ORCID: 0009-0003-5460-5208;
eLibrary SPIN: 3780-7865;
e-mail: AlexseyKryukov@yandex.ru

**Марюшин Леонид Александрович,**
канд. техн. наук, доцент,
профессор кафедры «Промышленная теплоэнергетика»;
ORCID: 0009-0000-5240-0186;
eLibrary SPIN: 3812-2917;
e-mail: katzbalger@yandex.ru

**Сенникова Ольга Борисовна,**
канд. техн. наук, доцент,
профессор кафедры «Промышленная теплоэнергетика»;
ORCID: 0009-0002-0069-5669;
eLibrary SPIN: 6470-5501;
e-mail: borjusya@yandex.ru

**Сёмочкин Глеб Викторович,**
студент кафедры «Менеджмент»;
ORCID: 0009-0000-4269-4678;
eLibrary SPIN: 3228-5831;
e-mail: glebsem03@gmail.com