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MODELS OF EFFECTIVE THERMAL CONDUCTIVITY OF BINARY COMPOSITE SYSTEMS

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Abstract. Methods for calculating the physical properties (thermal conductivity) of composite materials (CS) based on empirical and numerical models are investigated. These use the idea of Maxwell and Rayleigh about the proportionality of this parameter to the physical properties of the matrix and filler, as well as the concentration of the filler in the matrix. These models can consider the shape of the particles and their relative position. Comparison experimental data showed that such models are not universal and work only in the field of low concentrations of filler in the matrix. Another class of effective thermal conductivity models allows you to consider Thermal boundary resistance of the contact between the filler particles and the matrix (Kapitza thermal resistance). In this case, there is a serious problem of determining the thickness of the interfacial thermal layer, which can only be estimated by indirect methods. In general, the effective thermal conductivity of the composite (ETC) is also influenced by other factors: contact thermal resistance between filler particles, aggregation of filler particles, dependence of the physical properties of the filler on particle size, ordering of matrix molecules in the interfacial region. Numerical calculation is the most efficient because it is possible to consider the influence of a lot of factors, which is not possible in the case of an empirical model. A composite is a heterogeneous structure, so the generalized heat flux method is applicable. The average heat flux through the composite is calculated and then the effective thermal conductivity coefficient of the composite is calculated. The calculation of ETC is performed using the generalized heat flux method (GHFM). To solve the transient thermal conductivity equation, the Alternating Direction Implicit Method (ADI) was used. Methods for estimating the thickness of the Thermal boundary are proposed based on comparison of experimental data and the results of a computational experiment and considering the dimensional factor. The concentrations of the filler at which these factors have the greatest effect on the thermal conductivity of the composite have been determined. Software has been developed by applying the methods described.

Keywords: effective thermal conductivity, analytical models, numerical simulation, finite element analysis.

1. INTRODUCTION

The development of computational methods for effective thermal conductivity of composite systems was based on intuitively understandable dependencies of thermal conductivity on the concentration of the filler in the matrix, on the distribution of particles in the matrix, the geometry and orientation of the particles, the ratio of the thermal conductivity coefficients of the matrix and the filler, the clustering of filler particles, the ratio of particle sizes and the CS object, the interfacial thermal resistance (Kapitza resistance), and the contact thermal resistances between particles in a cluster. In general, this dependence can be represented by the expression [1].

$$\frac{\lambda_{eff}}{\lambda_1} = f\left(\frac{\lambda_2}{\lambda_1}, \rho_2, \frac{a}{L}, Bi\right) \quad (1)$$

λ_{eff} – ETC; λ_1 – thermal conductivity coefficient of the matrix; λ_2 – Thermal conductivity coefficient of the filler; ρ_2 – Bulk concentration of filler; a – Particle Radius; Bio Number $Bi = a/R_c\lambda_2$; L – Object size.

Let us consider the influence of these factors on ETC. In the field of our consideration will be polymer composites with a filler that has a higher thermal conductivity coefficient than the matrix. Such composites are in demand in systems where energy removal (cooling) is relevant, for example, electronic devices. The range of changes in the thermal conductivity coefficient of polymers used as a matrix is quite narrow from 0.1 to 0.4 W/(m·K). The range the coefficient of thermal conductivity of the filler is from 0.8 to 3000 W/(m·K). The task comes down to the need to obtain the maximum effective coefficient of thermal conductivity at specified materials of the matrix and filler. It is not easy to solve this problem experimentally, due to the influence of large number of factors including. The use of thermal conductivity modeling of a composite system can significantly speed up the process of creating a material with desired properties.

2. EMPIRICAL METHODS

Let's start with a review of empirical methods based on the Maxwell-Rayleigh model [2, 3]. Maxwell's model contains only the bulk concentrations and the thermal conductivity of the matrix and the filler, respectively, does not consider the structure of the filler, interfacial and contact thermal resistance, so it can only be used for preliminary estimates of the effective coefficient of thermal conductivity:

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{3\rho_2}{\frac{(\lambda_2 + 2\lambda_1)}{\lambda_2 - \lambda_1} - \rho_2} \right), \quad (2)$$

Rayleigh's model [3] considers the shape of the filler particles and their orientation: for spherical particles,

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{3\rho_2}{\frac{(\lambda_2 - 2\lambda_1)}{\lambda_2 - \lambda_1} - \rho_2 + \frac{1.569((\lambda_2 - \lambda_1))}{(3\lambda_2 - 4\lambda_1)} \rho_2^{3.33}} \right) \quad (3)$$

cylindrical particles located across the heat flow,

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{2\rho_2}{\frac{(\lambda_2 + \lambda_1)}{\lambda_2 - \lambda_1} - \rho_2 + \frac{(\lambda_2 - \lambda_1)}{(\lambda_2 - \lambda_1)(0.3058\rho_2^4 + 0.01336\rho_2^8)}} \right) \quad (4)$$

cylindrical particles located along the heat flow,

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{(\lambda_2 - \lambda_1)\rho_2}{\lambda_1} \right) \quad (5)$$

The Maxwell-Eucken model orients particles in the form of spheroids, cylinders, and plates:

$$\lambda_{eff} = \lambda_1 \left(1 + \frac{(\lambda_2/\lambda_1 - 1)L\rho_2}{1 + (L - 1)\rho_2} \right). \quad (6)$$

For spheroids ($f_1 = f_2 \neq f_3$), $L = \frac{1}{3} \sum_{i=1}^3 \left[1 + \left(\frac{\lambda_2}{\lambda_1} - 1 \right) f_i \right]^{-1}$, $\sum_{i=1}^3 f_i = 1$,

here are the semi-axes of the ellipsoid, f_i $L = (5\lambda_1 + \lambda_2)/[3(\lambda_1 + \lambda_2)]$ for the cylindrical shape of the filler particles, for the spherical shape of the filler particles; – for the lamellar form of filler particles. $L = 3\lambda_1/(2\lambda_1 + \lambda_2)$ $L = (\lambda_1 + 2\lambda_2)/3\lambda_1$

Fig.1 (2) plots relationships (2), (3), (6) and shows experimental data for ETC with an epoxy resin matrix at bulk concentrations less than 0.1. As demonstrated, the ETC remains virtually unchanged across different filler materials because of the absence of particle clusters. Consequently, the thermal conductivity of the matrix remains the primary controlling factor. This range is well described by models (3), (4), (6). Fig.1 (2) indicates that other models are needed for high concentrations of filler. Experimental data taken from [4, 5].

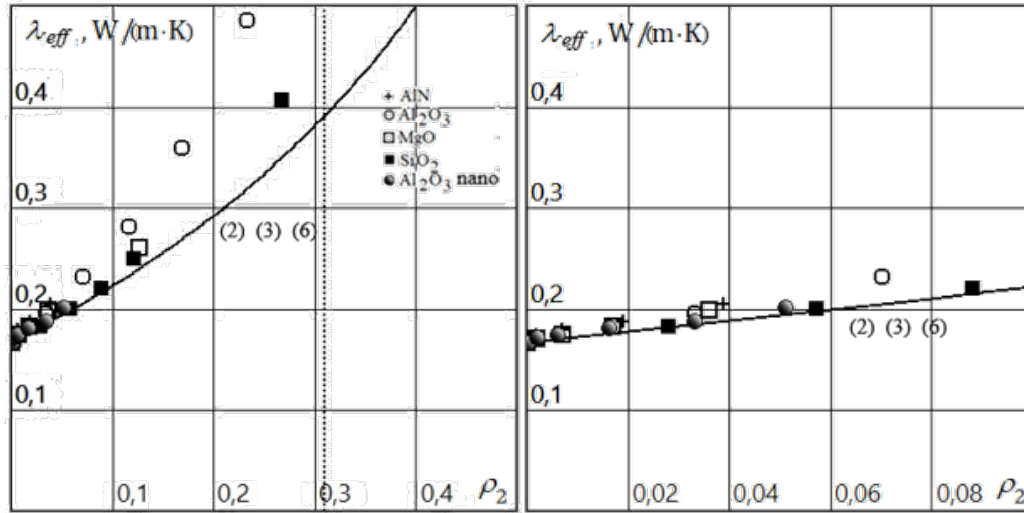


Figure 1 – ETC. The matrix is made of epoxy resin. 1. High concentrations of filler. 2. Low concentration of filler.

We consider two additional models to calculate the effective thermal conductivity coefficient, based solely on the filler volume fraction and the thermal conductivity of the matrix. The first is Odelevsky's model [6]:

$$\lambda_{\text{eff}} = \left(\frac{(3\rho_1 - 1)\lambda_1 + (3\rho_2 - 1)\lambda_2}{4} \right) + \left[\left(\frac{(3\rho_1 - 1)\lambda_1 + (3\rho_2 - 1)\lambda_2}{4} \right)^2 + \frac{\lambda_1\lambda_2}{2} \right]^{0.5}, \quad (7)$$

Lewis-Nielsen model [3]:

$$\lambda_{\text{eff}} = \lambda_1 \frac{1 + AB\rho_2}{1 - B\rho_2\psi} \quad (8)$$

$$B = \frac{\frac{\lambda_2}{\lambda_1} - 1}{\frac{\lambda_2}{\lambda_1} + A}; \quad \psi = 1 + \frac{1 - \rho_{2m}}{\rho_{2m}^2} \rho_2,$$

where A is the particle shape coefficient (1.5 – sphere), ρ_{2m} is the maximum particle packing (0.52).

As shown in Figure 2, the models align closely with the experimental data for aluminum oxide and silicon dioxide fillers, even at high concentrations. However, this agreement may be coincidental, given the lack of clear criteria to compare calculated and experimental values. Furthermore, exact experimental conditions are not always specified. The thermal conductivity of silicon dioxide, for example, can range from 0.02 to 10 W/(m·K) depending on its structural state. The experimental data are labeled as in Fig.1 (1). The considered models use the concentrations and thermal conductivities of the composite components as parameters. A more advanced approach is the Hasselman-Johnson

calculation method [7]. This account for the thermal resistance of the interfacial layer. For a spherical particle, the formula is:

$$\lambda_{eff} = \lambda_1 \frac{\left[2 \left(\frac{\lambda_2}{\lambda_1} - \frac{\lambda_2}{ah_c} - 1 \right) \rho_2 + \frac{\lambda_2}{\lambda_1} + \frac{2\lambda_2}{ah_c} + 2 \right]}{\left[\left(1 - \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} \right) \rho_2 + \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} + 2 \right]}, \quad (9)$$

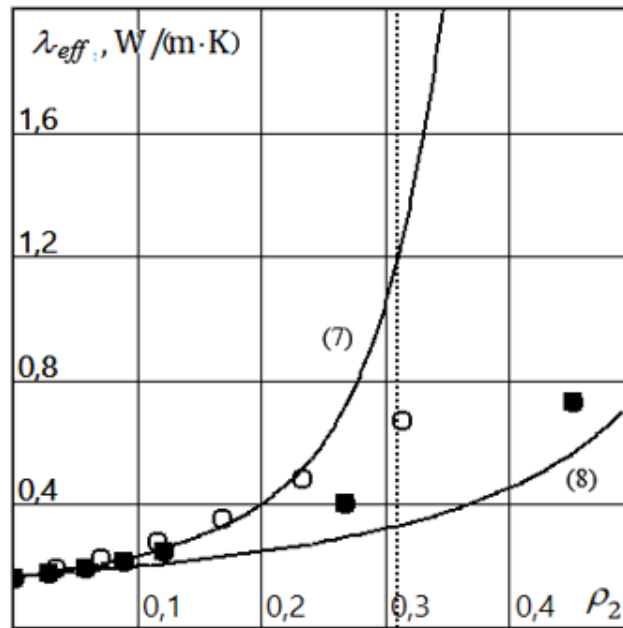


Figure 2 – Effective thermal conductivity of the epoxy-based composite. The solid lines represent the theoretical predictions by the Odelevsky (7) and Lewis-Nielsen models (8).

cylindrical,

$$\lambda_{eff} = \lambda_1 \frac{\left[\left(\frac{\lambda_2}{\lambda_1} - \frac{\lambda_2}{ah_c} - 1 \right) \rho_2 + \frac{\lambda_2}{\lambda_1} + \frac{2\lambda_2}{ah_c} + 1 \right]}{\left[\left(1 - \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} \right) \rho_2 - \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{ah_c} + 1 \right]} \quad (10)$$

plate,

$$\lambda_{eff} = \lambda_1 \frac{1}{\left[\left(1 - \frac{\lambda_2}{\lambda_1} + \frac{2\lambda_2}{ah_c} \right) \rho_2 + \frac{\lambda_2}{\lambda_1} \right]} \quad (11)$$

The Every and Tzou model belongs to the same category of models [3]:

$$(1 - \rho_2)^3 = \left(\frac{\lambda_1}{\lambda_{eff}} \right)^{(1+2\alpha)/(1-\alpha)} \left(\frac{\lambda_{eff} - \lambda_2(1-\alpha)}{\lambda_1 - \lambda_2(1-\alpha)} \right)^{3/(1-\alpha)} \quad (12)$$

where α – a coefficient that consider the particle size and interfacial thermal resistance, $\alpha = 2a_K/d$, where $a_K = \lambda_1/h_c$ is the Kapitza radius.

Fig.3 illustrates the empirical relationships of the equivalent thermal conductivity (ETC) for epoxy resin composites filled with aluminum oxide. Analyses of Figures 2 and 3 reveal that the Odelevsky and Hasselmann-Johnson models provide the best fit. However, these models differ significantly: the Odelevsky model relies solely on filler concentration, whereas the Hasselmann-Johnson model incorporates the properties of the interfacial layer. Estimates indicate that the thickness of the Kapitza

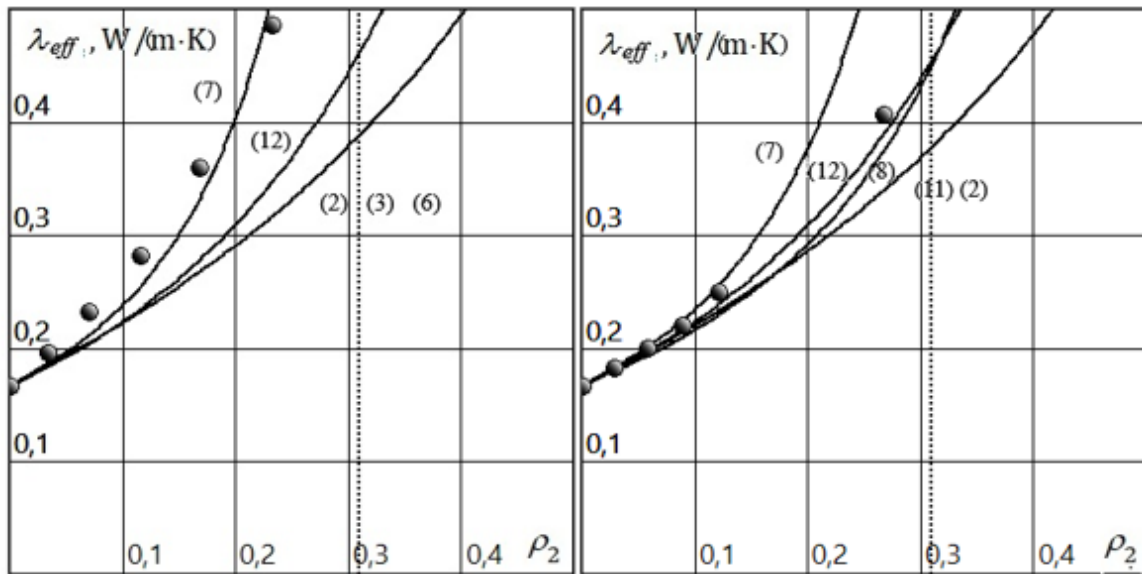


Figure 3 – Epoxy resin matrix with different fillers: 1) aluminum oxide (particle size of 4 μm); 2) silicon dioxide (particle size of 20 μm).

(interfacial) layer ranges from 2 to 16 nm [4], with the thermal boundary conductance of this layer reaching $10^8 \text{ W}/(\text{m}^2 \cdot \text{K})$.

Fig.4 presents a comparison between the experimental findings and the empirical models for the polyethylene–SiC and polyamide–SiC composites.

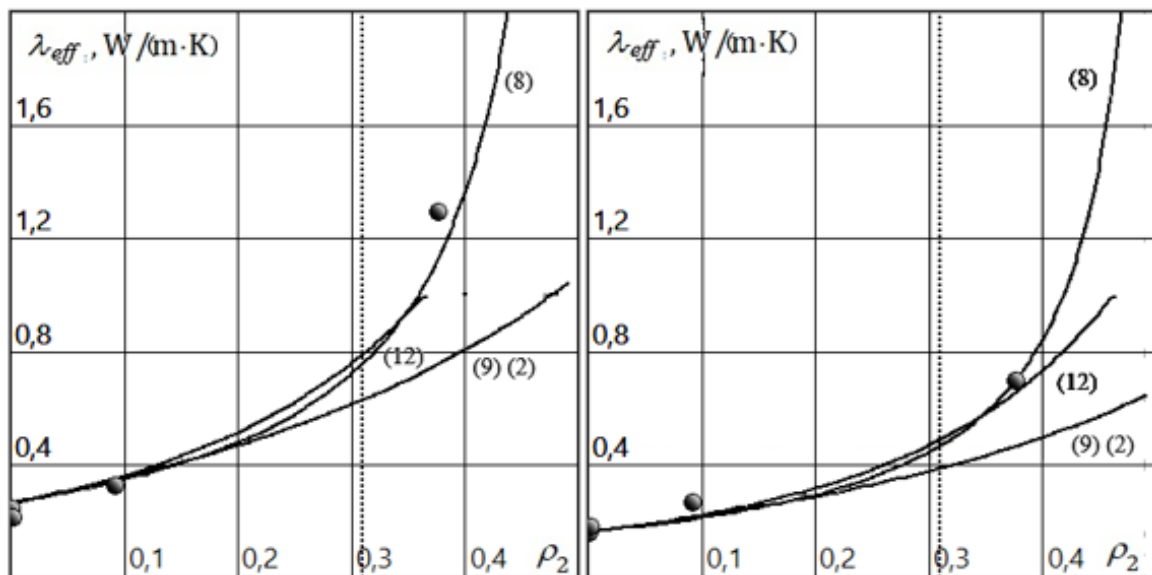


Figure 4 – 1) Polyamide–silicon carbide; 2) Polyethylene–silicon carbide; particle size 1 μm).

These models properly account for the interfacial thermal resistance. Nonetheless, the fundamental physics of energy transport at this interface requires further investigation.

Another frequently used model is the percolation model [8]:

$$\lambda_{\text{eff}} = \lambda_2 \left(\frac{\rho_1 - \rho_c}{1 - \rho_c} \right)^k, \quad (13)$$

$$\lambda_{\text{eff}} = \lambda_2 \left(\frac{\lambda_c}{\lambda_2} \right)^{\left(\frac{1-\rho_2}{1-\rho_c} \right)^k} \quad (14)$$

$k = 1.6, \rho_c = 0.15$.

This model includes a clustering parameter, ρ_c , which describes how particles clump together. In chaotic systems, particle clusters always form, causing contact resistance to add to interfacial resistance. At a volume concentration of roughly 0.311, a continuous chain of filler particles (a percolation cluster) forms, which dramatically increases conductivity. While this effect is vital for conductive metal fillers, we focus on dielectric fillers and omit percolation models. In all figures, the vertical dotted line corresponds to the concentration of the filler at the percolation threshold.

Fig.5 and 6 show the relative errors in the ETC calculation for different empirical models. The figures indicate that a calculation error of less than 10% is achieved only at filler concentrations of 0.1 or lower. Comparisons of empirical methods show they are only valid for dilute filler concentrations and preliminary ETC estimates. To account for a maximum number of influencing factors, numerical models must be used.

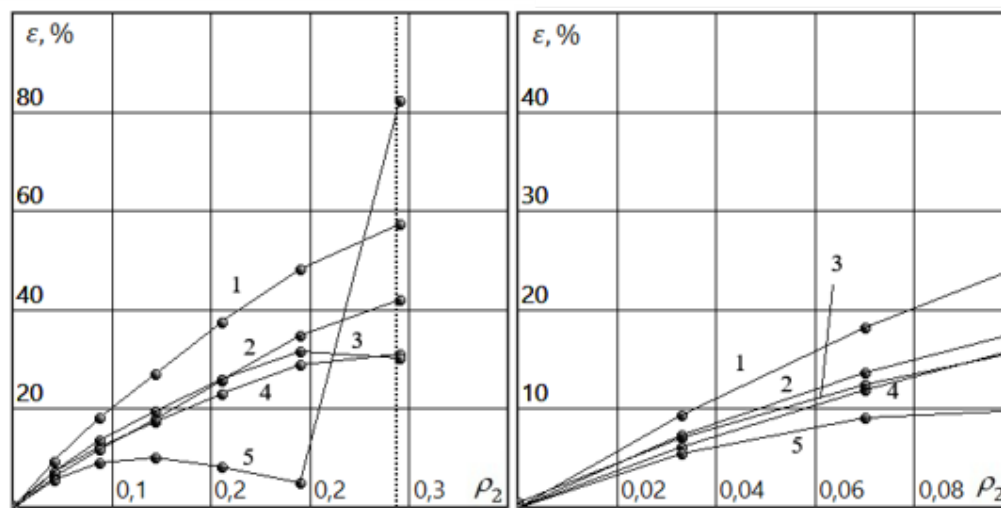


Figure 5 – Relative error of the thermal conductivity coefficient for the epoxy resin matrix with aluminum oxide (particle size of 4 μm). 1. Hasselmann-Johnson 2. Maxwell-Rayleigh. 3. Lewis-Nielsen. 4. Every-Tzow 5. Odelevsky.

3. NUMERICAL METHODS

We solve the transient heat conduction equation to determine the temperature field for the GHFM:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\lambda_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda_z \frac{\partial T}{\partial z} \right), \quad (15)$$

x, y, z – coordinates, m; ρ – density, kg/m^3 ; C_p – heat capacity; t – time, s; T – temperature, λ – Thermal Conductivity Coefficient, $\text{W}/(\text{m} \cdot \text{K})$.

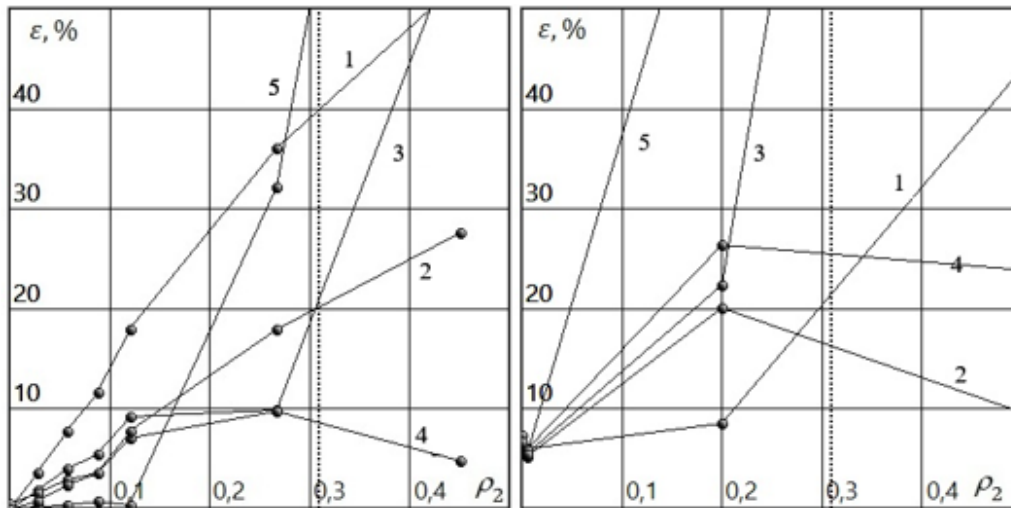


Figure 6 – Relative error in the effective thermal conductivity coefficient for (1) epoxy resin/SiO₂ (20 μm) and (2) polyamide/SiC (1 μm) composites. 1. Hasselmann-Johnson 2. Maxwell-Rayleigh. 3. Lewis-Nielsen. 4. Every-Tzow 5. Odelevsky.

The boundary conditions are shown (Fig. 7):

$$\begin{aligned}
 T &= T_b, \quad L_x \geq x \geq 0, \quad y = 0, \quad L_z \geq z \geq 0; \\
 T &= T_e, \quad L_x \geq x \geq 0, \quad y = L_y, \quad L_z \geq z \geq 0; \\
 T &= T_0, \quad L_x > x > 0, \quad L_y > y > 0, \quad L_z > z \geq 0; \\
 \frac{\partial T}{\partial x} &= 0, \quad \frac{\partial T}{\partial z} = 0, \quad x = 0, \quad x = L_x; \quad L_y > y > 0, \quad z = 0, \quad z = L_z,
 \end{aligned} \tag{16}$$

L_x, L_y, L_z – Linear dimensions of the element.

This problem was solved in [9, 10] by the relaxation method. In this work, the ADI (Alternating Direction Implicit) method of fractional steps is applied [11, 12]. The finite-difference representation of equation (15) is approximated by the unconditionally stable implicit scheme [13].

$$\rho C_p \frac{T_{ijk}^{n+1} - T_{ijk}^n}{\Delta t} = \sum_{m=i,j,k} \frac{\Theta [\delta(\lambda \delta T_{ijk})]_m^{n+1} + (1 - \Theta) [\delta(\lambda \delta T_{ijk})]_m^n}{(\Delta h)^2}, \tag{17}$$

where

$m = i, j, k$;

$i = 1 \dots N_x, j = 1 \dots N_y, k = 1 \dots N_z$;

$n = 0, 1, 2 \dots$ – time step index;

Δh – the step of splitting by coordinates (we assume the same along the x, y and z axes);

$0 \leq \Theta < 1$ – Weighting coefficient.

When $m = i$, the expression for $[\delta(\lambda \delta T_{ijk})]_i^{n+1}$ is written as:

$$[\delta(\lambda \delta T_{ijk})]_i^{n+1} = \lambda_{i+\frac{1}{2}} (T_{i+1,jk}^{n+1} - T_{ijk}^{n+1}) - \lambda_{i-\frac{1}{2}} (T_{ijk}^{n+1} - T_{i-1,jk}^{n+1}) \tag{18}$$

The system of equations (16) can be rewritten using matrix difference operators with variable coefficients considering (17):

$$T_{ijk}^{n+1} - T_{ijk}^n = \Theta (\Lambda_1 T^{n+1} + \Lambda_2 T^{n+1} + \Lambda_3 T^{n+1}) + (1 - \Theta) \Lambda_1 T^n + \Lambda_2 T^n + \Lambda_3 T^n \tag{19}$$

where $\Lambda_1, \Lambda_2, \Lambda_3$ – matrix difference operators with variable coefficients.
Apply these operators to the expression (19):

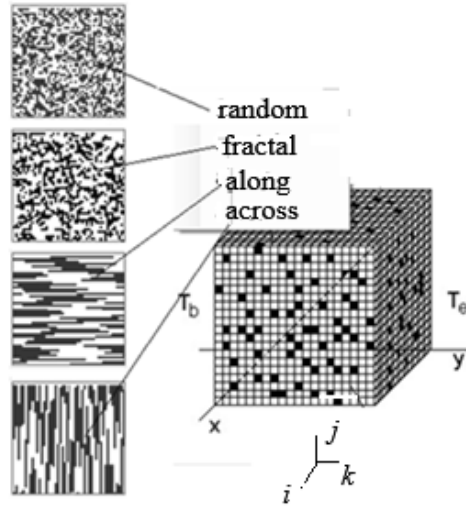


Figure 7 – On formulating a mathematical problem.

$$\Lambda_1 T^d = \text{Fo}_{i+1/2} T_{i+1,jk}^d - (\text{Fo}_{i+1/2} + \text{Fo}_{i-1/2}) T_{ijk}^d + \text{Fo}_{i-1/2} T_{i-1,jk}^d, \quad (20)$$

$$\Lambda_2 T^d = \text{Fo}_{j+1/2} T_{i,j+1,k}^d - (\text{Fo}_{j+1/2} + \text{Fo}_{j-1/2}) T_{ijk}^d + \text{Fo}_{j-1/2} T_{i,j-1,k}^d, \quad (21)$$

$$\Lambda_3 T^d = \text{Fo}_{k+1/2} T_{i,j,k+1}^d - (\text{Fo}_{k+1/2} + \text{Fo}_{k-1/2}) T_{ijk}^d + \text{Fo}_{k-1/2} T_{i,j,k-1}^d, \quad (22)$$

where $d = n + 1$ or $d = n$.

$1 \leq i \leq N_x, 1 \leq j \leq N_y, 1 \leq k \leq N_z$ – coordinates indices; Δt – time step, s; Δh – step by coordinates, m;

N_x, N_y, N_z – Number of nodes on the x, y, z axes. Fourier number:

$$\text{Fo}_{m+1/2} = \frac{\lambda_{m+1/2} \Delta t}{\rho C_p \Delta h^2}; \quad \text{Fo}_{i-1/2} = \frac{\lambda_{m-1/2} \Delta t}{\rho C_p \Delta h^2};$$

$$\lambda_{m\pm 1/2} = \frac{2}{\frac{1}{\lambda_{1(m\pm 1)}} + \frac{1}{\lambda_{2(m\pm 1)}} + \frac{2}{K_c \Delta h}} \quad \text{– particle-matrix contact,}$$

$$\lambda_{m\pm 1/2} = \frac{1}{\frac{1}{\lambda_{2(m\pm 1)}} + \frac{1}{K_p \Delta h}} \quad \text{– particle-to-particle contact,}$$

K_c – thermal conductivity of the particle-matrix contact (interfacial contact),

K_p – thermal conductivity of particle-to-particle contact.

$C_p = \frac{C_1 + C_2}{2}$ – Average heat capacity of contacting elements,

The system of equations (19) can be solved by the method of fractional steps [11, 12]. For this purpose, the time-step discretization is defined as follows:

$$-\Theta \Lambda_1 T^{n+1/3} + T_{ijk}^{n+1/3} = (1 - \Theta) \Lambda_1 T^n + T_{ijk}^n \quad (23)$$

$$-\Theta \Lambda_2 T^{n+2/3} + T_{ijk}^{n+2/3} = (1 - \Theta) \Lambda_2 T^{n+1/3} + T_{ijk}^{n+1/3} \quad (24)$$

$$-\Theta \Lambda_3 T^{n+1} + T_{ijk}^{n+1} = (1 - \Theta) \Lambda_3 T^{n+2/3} + T_{ijk}^{n+2/3}, \quad (25)$$

The main time step Δt is divided into three intervals: the index $n + 1/3$ corresponds to the moment in time $t_{n+1/3} = t_n + 1/3\Delta t$, $t_{n+2/3} = t_n + 2/3\Delta t$, $t_{n+1} = t_n + \Delta t$. Equations (23)–(25) are solvable at a single timestep via the forward-backward sweep method. The solution procedure is detailed below using equation (23) as an example. The tridiagonal matrix algorithm is applied. To proceed, group the terms associated with moments n and $n + 1/3$.

$$-\Theta(\text{Fo}_{i+1/2/3})T_{i+1,jk}^{n+1/3} + (1 + \Theta\text{Fo}_{i+1/2/3} + \Theta\text{Fo}_{i-1/2/3})T_{ijk}^{n+1/3} - \Theta T_{i-1,jk}^{n+1/3}\text{Fo}_{i-1/2/3} = G_i \quad (26)$$

$$G_i = (1 - \Theta)\Lambda_1 T^n + T_{ijk}^n.$$

Let's rewrite (26) considering the new designations:

$$A_i = \Theta(\text{Fo}_{i+1/2/3}); B_i = 1 + \Theta\text{Fo}_{i+1/2/3} + \Theta\text{Fo}_{i-1/2/3}; C_i = \Theta\text{Fo}_{i-1/2/3},$$

$$-A_i T_{i+1,jk}^{n+1/3} + B_i T_{ijk}^{n+1/3} - C_i T_{i-1,jk}^{n+1/3} = G_i \quad (27)$$

A solution to Equation (27) is sought in the form:

$$T_{ijk}^{n+1/3} = E_i T_{i+1,jk}^{n+1/3} + F_i \quad (28)$$

Replace in (27) $T_{i-1,jk}^{n+1/3}$ using expression (28), resulting in:

$$E_i = \frac{A_i}{B_i - C_i E_{i-1}} \quad (29)$$

$$F_i = \frac{G_i - C_i F_{i-1}}{B_i - C_i E_{i-1}} \quad (30)$$

From the boundary condition $i = 1$ where $\frac{\partial T}{\partial x} = 0$, we obtain:

$$E_0 = 1, \quad F_0 = 0 \quad (31)$$

Using (29)–(31), we can calculate by induction in the ascending direction E_i and F_i , and then from expression (27) we find the temperatures $T_{ijk}^{n+1/3}$. Equations (24) and (25) are solved in the same way. The only difference lies in the starting values of E_i F_i . From the boundary condition $k = 1$ where $T_{1,jk} = T_b$, we obtain:

$$E_0 = 0, \quad F_0 = T_b, \quad (32)$$

From the boundary condition $j = 1$ where $\frac{\partial T}{\partial z} = 0$, we obtain:

$$E_0 = 1, \quad F_0 = 0 \quad (33)$$

As a result, the temperatures in all nodes of the grid for the current time step will be obtained. Average heat flux through sample:

$$q_{avi} = \frac{1}{N_x(N_y - 1)N_z} \sum_{j=1}^{N_z} \sum_{k=1}^{N_y-1} \sum_{i=1}^{N_x} \lambda_{ij,k+1/2} \frac{(T_{ijk+1} - T_{ijk})}{\Delta h} \quad (34)$$

The effective thermal conductivity coefficient of the composite is calculated by the following equation:

$$\lambda_{eff} = \frac{q_{avi} \cdot L_x}{T_e - T_b} \quad (35)$$

The software was developed to implement equations (18)–(35). To verify the algorithm, we simulated the temperature distribution in a homogeneous sample under specific boundary conditions (16). The initial temperature distribution along the y-axis was assumed to be linear. Other parameters had the following values: time step $\Delta t = 10^{-6}$ s, coordinate step, temperature interval, thermal conductivity coefficient of the material, weight coefficient $\Delta h = 10^{-5}$ m, $T_e - T_b = 200$ K, $\lambda = 40$ W/(m · K), $\Theta = 0.5$ (Crank–Nicolson scheme), random distribution of the filler in the matrix. The remaining parameters were defined as follows: time step $\Delta t = 10^{-6}$ s, coordinate step $\Delta h = 10^{-5}$ m, temperature interval $T_e - T_b = 200$ K, thermal conductivity of the material = 40 W/(m · K) and weight coefficient $\Theta = 0.5$ (Crank–Nicolson scheme). The filler was assumed to be randomly distributed within the matrix. The thermal conductivity coefficient of the material was calculated $\lambda = 39.998$ W/(m · K), with the temperature determination error not exceeding 0.5%. Similar results were obtained using a purely implicit scheme, where $\Theta = 1$.

The composite structure is generated on a volumetric lattice with dimensions $L_x \times L_y \times L_z$. After setting the volumetric concentration of the filler, the number of cells per filler particle is calculated. The required distribution of the filler within the matrix is then generated (Fig. 7). Figure 8 presents the numerical calculations and compares them with experimental data regarding the effective thermal conductivity coefficient. The value of interfacial thermal resistance $R_c = 1/K_c$ was determined by expression (40). The thermal resistance of the particle-to-particle contact $R_p = 1/K_p$,

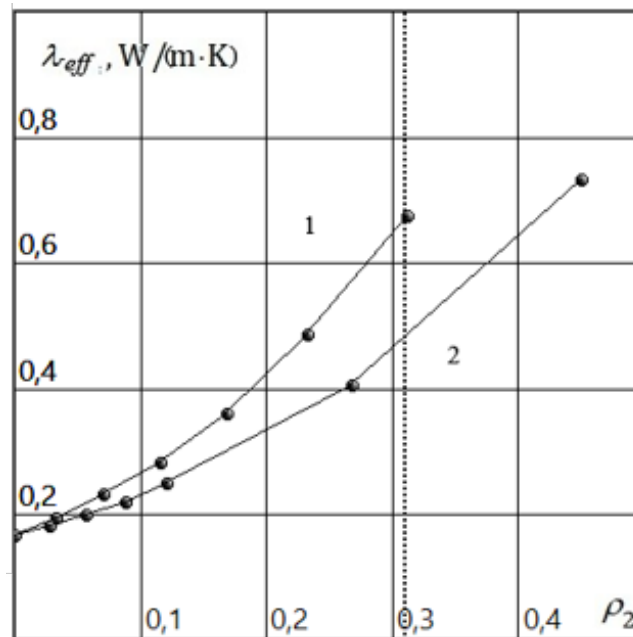


Figure 8 – Epoxy resin matrix: 1. aluminum oxide (particle size of 4 μm); 2. silicon dioxide (particle size of 20 μm); Points – experiment, lines – numerical calculations.

The developed software enables the generation of various filler distributions within the matrix (Fig. 7). The influence of these distributions on the effective thermal conductivity (ETC) is depicted in Fig. 8.

Next, we will briefly discuss the factors that complicate the calculation of thermal conductivity in composites.

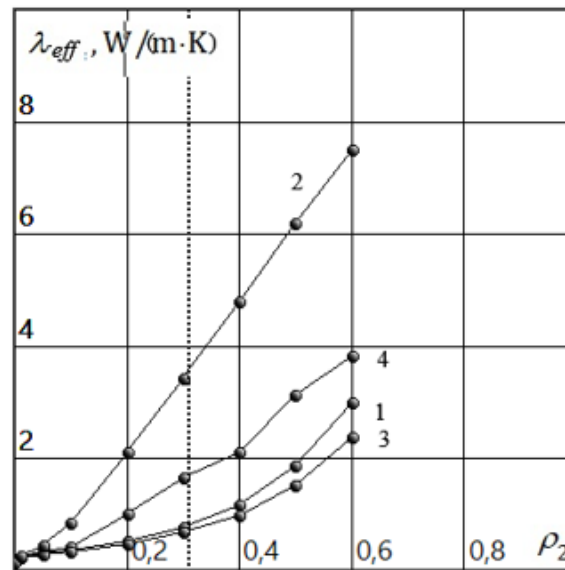


Figure 9 – Effective thermal conductivity (ETC) for polyethylene–silicon carbide structures with various orientations: (1) randomly oriented, (2) longitudinal, (3) transverse, and (4) fractal.

4. FACTORS

4.1. Matrix modification

We can increase the thermal conductivity of a matrix by raising its degree of crystallinity. When adding a modifier to the matrix, we assume for preliminary evaluation that the entire interfacial region becomes crystalline. Under this assumption, any increase in the overall degree of crystallinity depends on two factors: the particle–matrix contact area and the thickness of the interfacial region. Fig. 9 presents these relationships. Fig. 10-1 plots the contact area between the particles and the matrix, as well as the clustering coefficient. Fig. 10-2 shows that the degree of crystallinity rises with longer filler concentrations. As we can see, within standard operating concentrations, the filler only causes a very small increase in crystallinity at the interfacial layer.

4.2. Size effects

On the one hand, decreasing the filler particle size increases the interfacial surface area at any given concentration. This increases the relative proportion of crystallites in the matrix due to inoculation compared to the amorphous fraction, which generally raises the effective thermal conductivity of the matrix. On the other hand, a smaller particle size can reduce thermal conductivity due to phonon scattering at particle boundaries. Fig. 11 presents experimental dependencies [3] of the effective thermal conductivity, which clearly demonstrate the influence of this dimensional factor.

Paper [14] discusses how thermal conductivity depends on the size factor and examines energy transfer mechanisms in nanosystems. Furthermore, paper [15] explains the influence of particle size on the thermal conductivity coefficient. This effect occurs due to shifting energy transfer mechanisms in small particles, namely diffusion and ballistic transport [16].

$$\lambda_{eff} = \frac{1}{3} \sum_i \int k_B (\hbar \omega_i / (k_B T))^2 \frac{\exp(\hbar \omega_i / (k_B T))}{\exp \hbar \omega_i / (k_B T) - 1} v_i(k) l_i(k) \cos^2 \Theta dk, \quad (36)$$

where:

k_B – Boltzmann constant; k – the angular deviation between the wave vector and the energy flow; ω_i

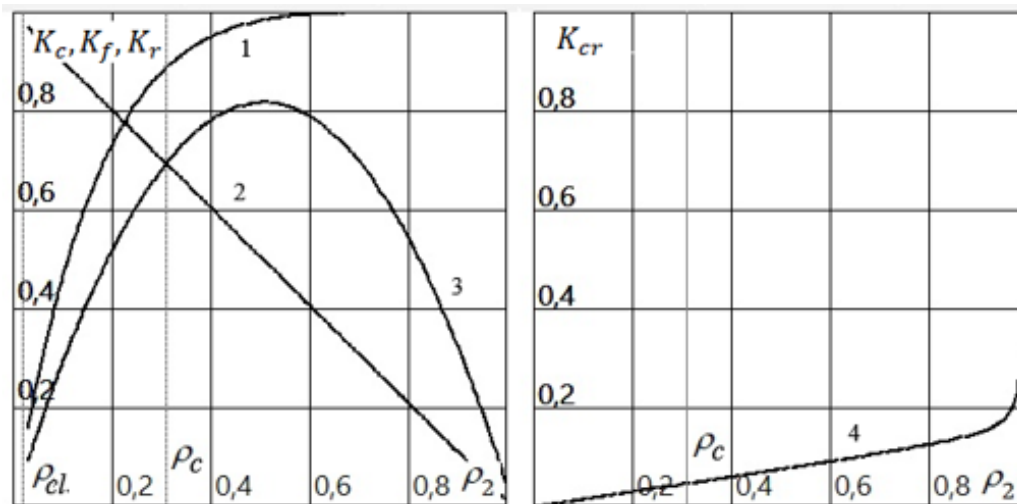


Figure 10 – Clustering coefficients

1. $K_c = N_c/N$ – Clustering coefficient; 2. $K_f = F_m/F_f$ – contact ratio; 3. $K_r = F_m/F_c$ – particle–matrix contact coefficient; 4. $K_{cr} = V_{cr}/V$ – degree of crystallinity; F_f – Total surface area of particles; F_c – Particle–matrix contact area at the percolation threshold; N_c – Number of particles in clusters; N – Total number of filler particles; ρ_c – Percolation threshold; ρ_{cl} – Clustering threshold, the critical concentration for the onset of clustering; V_{cr} – Volume of the crystalline phase of the polymer; V – Total polymer volume.

– the frequency, v_i – group velocity, τ_i – phonon relaxation time, $\hbar$ – Planck-Dirac constant.

Usually, the nanoscale range is defined as up to 100 nm. However, this threshold varies by substance. The unique physical properties of a material appear when the number of internal atoms is roughly equal to the number of surface atoms. Additionally, for dielectrics and semiconductors, the phonon mean free path (the average distance a particle travels before it collides) is a key factor. Therefore, we can use this distance as the maximum limit of nanoscale size for these materials.

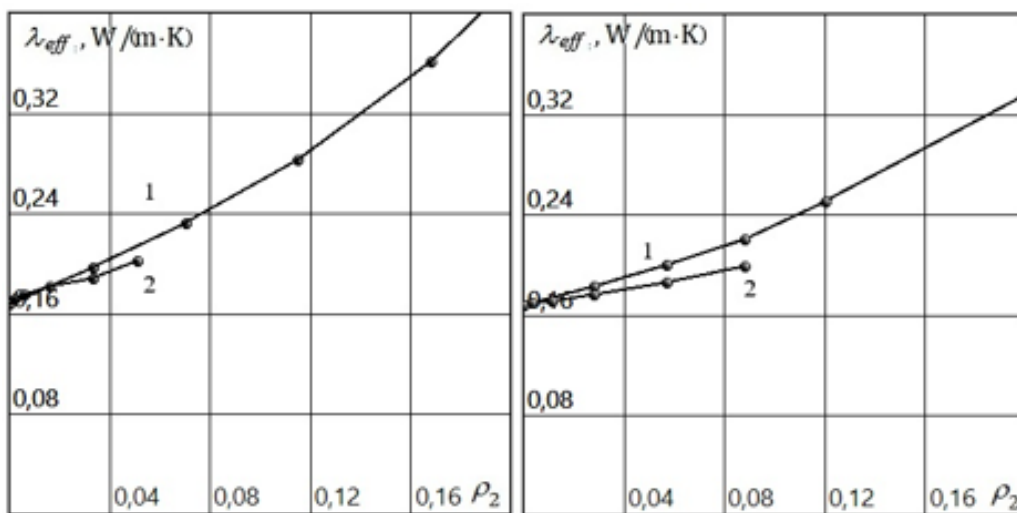


Figure 11 – Experimental dependencies of effective thermal conductivity (ETC) on filler particle size, 1) Epoxy resin + Al_2O_3 at particle sizes: $4\ \mu\text{m}$ (1) and $30\ \text{nm}$ (2); 2) Epoxy resin + SiO_2 at particle sizes of $20\ \mu\text{m}$ (1) and $20\ \text{nm}$ (2).

Heat transfer occurs via two primary mechanisms: diffusive and ballistic. These regimes depend on the Knudsen number. Furthermore, the particle-size-dependent thermal conductivity can be

expressed by a simple formula [14]:

$$\lambda_s = \frac{\lambda_0}{1 + Kn}, \quad Kn = \frac{l}{a}; \quad (37)$$

By substituting the phonon mean free path values into equation (1) and varying the particle size, we can determine how the material's thermal conductivity depends on particle dimensions (see Fig. 11).

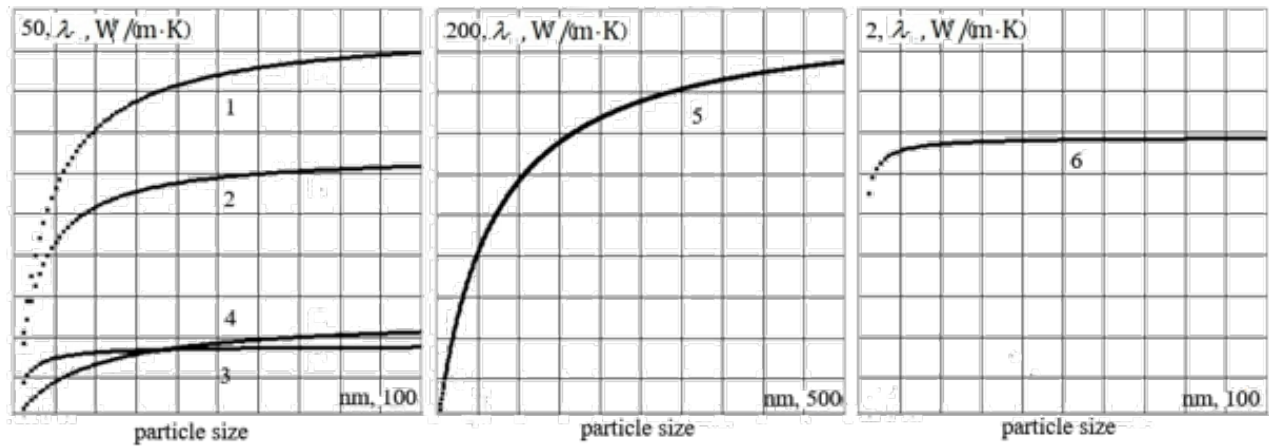


Figure 12 – Dependence of the effective thermal conductivity (ETC) of a particle on its size: 1 – MgO; 2 – Al₂O₃; 3 – TiO₂; 4 – ZnO; 5 – SiC; 6 – SiO₂.

Fig. 12 illustrates that the maximum limit of the nanoscale range, beyond which thermal conductivity remains constant, differs among substances. Furthermore, a reduction in the effective thermal conductivity of the composite relates to an increase in particle-matrix interfacial contacts.

4.3. Interfacial Region

It is well established that a thermal resistance (Kapitza resistance) occurs at the interface of two dissimilar materials, even when the solids are in perfect contact [17]:

Thermal resistance between phases is determined by the interfacial structure and the physicochemical interaction (adhesion) between the matrix and the filler. At the same time, there are practically no simple formulas to determine the thickness of the interfacial layer [18]:

$$\delta_f = \lambda_1 \frac{D_c}{2} \left\{ 1 - \rho_{fp}^{-1/3} \left[\frac{1}{11} \left(\frac{E_c}{E_1} - 1 \right) \right]^{1/1.7} \right\} \quad (38)$$

E_c, E_1 – the modulus of elasticity of the composite and the matrix, respectively;

ρ_{fp} – unaggregated filler volume fraction.

The application of these formulas is limited by the need to know several parameters that are difficult to determine experimentally (e.g., polymer-particle interfacial tension and polymer melt viscosity).

In [19], the interfacial thermal resistance of finely dispersed fillers is combined with the intrinsic thermal resistance of the particles. Consequently, the thermal conductivity coefficient of the filler, λ_n , is replaced by an effective thermal conductivity coefficient, λ_{neff} .

$$\lambda_{neff} = \frac{\lambda_n}{1 + \frac{R_{K1n}}{d_n}} \quad (39)$$

d_n – mean filler particle size,

By adjusting the thermal interfacial resistance, we achieved alignment between the theoretical and experimental curves. Experimental data indicates that a composite with an Al_2O_3 filler concentration of 0.312 exhibits an effective thermal conductivity (ETC) of $0.675 \text{ W}/(\text{m} \cdot \text{K})$. Because direct experimental methods to determine Kapitza thermal layer parameters—such as thermal resistance and thickness—are currently unavailable, we evaluated combined analytical and numerical approach. One such variant is detailed in. Given reliable experimental ETC data for a composite, numerical simulations can be performed using the Kapitza layer's thermal resistance as a fitting parameter. When the experimental and calculated ETC values match, the thickness of the Kapitza thermal layer is determined using its thermal resistance and effective thermal conductivity. In this study, optimal convergence was achieved at a thermal resistance of $10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$, yielding a Kapitza layer thickness of 6.75 nm. This value is consistent with the literature, where reported thermal interfacial layer thicknesses range from 1 to 22 nm.

Research [20] explores methods to determine the effective thermal conductivity (ETC) of epoxy composites filled with carbon nanotubes. These studies confirm that adding a highly thermally conductive filler does not guarantee a high overall ETC for the composite. The main challenge is the poor thermal transfer between filler particles. This issue occurs because of interfacial thermal resistance and contact resistance between the nanotubes. The thermal contact resistance for overlapping nanotubes is $6.46 \cdot 10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$ across a 2.5 nm distance. Other simulations estimate this value at $8.3 \cdot 10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$. These values were found for nanotubes that are 6 nm in diameter and 8 nm to 40 nm in length. Additionally, thermal resistance increases sharply when the gap between fibers exceeds 10 Å. Reference [21] further explains why highly conductive composites are difficult to achieve, even with carbon nanotube fillers. Finally, research [22] shows that thermal resistance is higher when nanotubes are arranged longitudinally (end-to-end) compared to a transverse (side-by-side) fiber arrangement.

The assessment of the interfacial thermal resistance can be made according to the acoustic mismatch model [23]:

$$R_c = \frac{2(\rho_1 v_1 + \rho_2 v_2)^2}{C_1 \rho_1^2 v_1^2 \rho_2 v_2} \left(\frac{v_2}{v_1} \right)^2 \quad (40)$$

Equation (40) yields interfacial thermal resistance values on the order of 10^{-8} for the composites considered above $10^{-8} \text{ m}^2 \cdot \text{K}/\text{W}$.

5. CONCLUSIONS

Preliminary calculations of the effective thermal conductivity (ETC) in composites significantly reduce the labor required to develop materials with specific physical properties. However, classical empirical models struggle to adapt to unique compositional systems, particularly at filler concentrations below 0.1%. Numerical methods offer the most successful approach, as they can account for a wide variety of variables. Consequently, increasing the ETC of polymer-based composites for electronic heat dissipation depends on multiple design factors (Table 1).

Although the high thermal conductivity of fillers increases the effective thermal conductivity (ETC) of polymer composites, this effect is only significant at concentrations above the percolation threshold (0.311). Unlike the sharp increase observed in electrical hopping conductivity, experimental and numerical evaluations of the effective thermal conductivity show no such jump. This is because contact thermal resistance increases as particle clusters grow. According to the tabulated data, the filler's intrinsic thermal conductivity mainly plays a role at relatively high values. While filler particles alter the boundary layer by increasing its thermal conductivity, the total volume of this

Table 1. Factors Affecting the Effective Thermal Conductivity of a CS.

Factor	$\rho_2 = 0.5\%$	$\rho_2 = 20\%$	$\rho_2 = 60\%$
Thermal conductivity of the matrix	+	+	—
Thermal conductivity of the filler	—	+	+
Modification	+	—	—
Filler agglomerates	—	+	+
Interfacial Contact		+	—
Contact resistance of filler particles	—	+	+
Size effects		+	+

interfacial space is too small to significantly affect the overall ETC. Furthermore, the Kapitza thermal resistance—the temperature drops at the interface between the filler and the matrix—acts as a barrier. Together with the thermal resistance between the particles within the cluster, this resistance prevents a major increase in composite ETC, even when highly conductive fillers (like carbon nanotubes) are used.

The following factors exert a decisive impact on the effective thermal conductivity of the composite and warrant further investigation: the manufacturing technique of the composite, the clustering and percolation structuring of the filler within the matrix, and the interfacial thermal contact resistance between the filler particles.

At low filler concentrations (until clusters are formed), the effective thermal conductivity is completely determined by the properties of the matrix. In fact, at low concentrations, the ratio of the effective thermal conductivity to the thermal conductivity of the matrix $K = \lambda_{eff}/\lambda_1$ is a characteristic of the modifier. The concentrations of the filler at which the factors affecting the effective thermal conductivity (thermal conductivity of the matrix, thermal conductivity of the filler, inoculation, clustering of the filler, interfacial resistance, contact resistance of filler particles) are significant.

At low filler concentrations—before filler clusters or continuous networks form—the effective thermal conductivity is determined entirely by the properties of the matrix. In fact, the ratio of the effective thermal conductivity to the matrix's thermal conductivity $K = \lambda_{eff}/\lambda_1$ serves as a primary characteristic of the modifier at these low concentrations. However, as filler concentration increases, several additional factors become significant in determining the effective thermal conductivity.

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A COMPARATIVE STUDY OF EXPERIMENTAL AND THEORETICAL MODELS OF MUTUAL DIFFUSION COEFFICIENTS IN HYDROCARBON GAS MIXTURES AT DIFFERENT TEMPERATURES

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Abstract. This article examines the problems of determining and comparing mutual diffusion coefficients of binary gas mixtures in the temperature range of 273–373 K at atmospheric pressure. The characteristic features of experimental data presented in the classical compilation by Marrero & Mason are analyzed and compared with calculated values obtained using the semi-empirical Fuller method and the kinetic-theoretical Chapman–Enskog method. The necessity of refining the temperature dependences of diffusion coefficients for systems involving hydrocarbon and non-hydrocarbon gases used in oil and gas and energy processes is substantiated. Based on the analysis, the author shows that the applied models reflect experimental trends to varying degrees: the Chapman–Enskog method better describes light gas mixtures, whereas the Fuller correlation provides satisfactory agreement for heavier hydrocarbons. Conclusions are drawn regarding the applicability ranges of each approach, and the practical significance of the results for mass transfer calculations in engineering models and numerical simulations of diffusion processes is highlighted.

Keywords: diffusion coefficients, hydrocarbon gases, Chapman–Enskog theory, Lennard-Jones potential, Fuller method, gas mixtures, mass transfer.

1. INTRODUCTION

Mutual diffusion processes play a key role in mass transfer and thermophysical phenomena that determine the behavior of multicomponent gas mixtures in chemical engineering, energy systems, and natural environments. Mutual diffusion coefficients (D_{12}) are important transport properties required for the accurate description of combustion, mixing, distillation, absorption, and other technological processes. The accuracy of their determination directly affects the reliability of engineering calculations and the results of numerical simulations in software packages [1, 3, 4].

Despite the long history of studying diffusion phenomena, the issue of reconciling experimental data with theoretical and semi-empirical models remains relevant. For most binary mixtures, especially those containing hydrocarbons, significant discrepancies are observed between the calculated and measured coefficients. This is due to differences in experimental techniques and the limitations of theoretical approaches, which do not always adequately account for the molecular features of components and the influence of temperature and pressure [2, 5].

Classical work by Chapman and Enskog laid the foundation for the kinetic-theory description of diffusion, enabling the calculation of coefficients based on intermolecular interaction potentials and effective particle diameters. However, the practical application of these formulas is complicated by the need to know potential parameters, which are often unavailable for complex molecules. In turn, the semi-empirical Fuller method, based on the concept of diffusion volumes, has become widely used in engineering calculations due to its simplicity and satisfactory accuracy for a wide range of gases. Nevertheless, its predictive accuracy decreases when moving from light inorganic systems to hydrocarbon mixtures, where the effects of molecular polarizability and anisotropy become significant.

Comprehensive compilations of experimental data, such as those presented in [3], as well as modern NIST databases, provide systematized information on D_{12} for hundreds of binary systems, including hydrocarbon gases, carbon dioxide, nitrogen, hydrogen and other technologically important components [3, 6, 7, 8, 9]. These databases serve as a foundation for validating and refining theoretical and correlation models. However, analysis shows that even under standard conditions ($T = 273\text{--}373\text{ K}$, $p = 1\text{ atm}$), noticeable discrepancies between experimental and calculated values persist, which require a comprehensive reassessment of existing approaches and clarification of their applicability limits.

The present work is devoted to a comparative study of mutual diffusion coefficients for a number of binary gas mixtures, including both hydrocarbon and non-hydrocarbon components. Experimental data from Marrero and Mason are used as the reference, while the Chapman–Enskog method and the semi-empirical Fuller correlation are applied for calculations. Seven gas pairs are considered: $\text{CH}_4\text{--C}_2\text{H}_6$, $\text{CH}_4\text{--C}_3\text{H}_8$, $\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$, $\text{CH}_4\text{--CO}_2$, $\text{CO}_2\text{--N}_2$, $\text{CH}_4\text{--N}_2$, and $\text{C}_3\text{H}_8\text{--N}_2$, covering a wide range of molecular masses and structural characteristics.

The aim of this study is to determine the degree of agreement between theoretical and semi-empirical models and experimental data in the temperature range $273\text{--}373\text{ K}$ at atmospheric pressure, to identify trends in the temperature dependence of D_{12} , and to propose recommendations for selecting the most appropriate calculation methods for engineering applications. In the course of the work, experimental and calculated $D(T)$ dependencies are analyzed, graphical relationships are constructed, and relative deviations between models and experimental data are evaluated. The results obtained make it possible to assess the accuracy of commonly used methods for calculating mutual diffusion coefficients and to determine the ranges in which each model provides the best agreement with experimental data [2, 4, 12, 13].

Thus, this article is aimed at a comprehensive comparison of three approaches—experimental, theoretical, and semi-empirical—applied to real gas systems, which is of practical importance for modeling mass transfer processes in the chemical and oil and gas industries, as well as for developing thermodynamic models for multicomponent mixtures.

2. METHODOLOGY

The study is based on a comparative analysis of mutual diffusion coefficients of binary gas systems with the aim of comparing experimental data and calculation results obtained using two widely applied methods — the semi-empirical Fuller method and the kinetic-theoretical Chapman–Enskog method. The choice of these approaches is justified by the fact that they represent two conceptually different but widely used classes of models: the former is based on correlation relationships and experimentally fitted parameters, while the latter relies on the fundamental theory of gas kinetics and intermolecular interaction potentials.

Seven binary gas pairs were selected as the systems under study: $\text{CH}_4\text{--C}_2\text{H}_6$, $\text{CH}_4\text{--C}_3\text{H}_8$, $\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$, $\text{CH}_4\text{--CO}_2$, $\text{CO}_2\text{--N}_2$, $\text{CH}_4\text{--N}_2$, and $\text{C}_3\text{H}_8\text{--N}_2$. These mixtures cover a wide range of molecular masses, sizes, and types of interactions, including nonpolar, weakly polar, and asymmetric combinations of components. Such a selection ensures the representativeness of the analysis for real technological conditions—from natural gas and associated petroleum gases to mixtures encountered in combustion and separation processes. The temperature range of $273\text{--}373\text{ K}$ and a pressure of 1 atm were chosen as the most relevant for engineering calculations and thermodynamic modeling under standard conditions.

Experimental values of the mutual diffusion coefficients D_{12} for the seven binary gas systems were taken from critically evaluated compilations [3, 11], which summarize the most reliable measurements

performed in the temperature range from 273 to 373 K at atmospheric pressure. The values are given in cm^2/s and are reduced to standard conditions (1 atm). For intermediate temperatures not available in the original sources, a power-law approximation of the temperature dependence, $D \propto T^{1.75}$, was used, which corresponds to empirical diffusion trends in dilute gases. The summarized experimental data used in the subsequent comparative analysis are presented in Table 1.

Table 1. Experimental mutual diffusion coefficients of binary gas mixtures at 1 atm in the temperature range 273–373 K [3, 11]

№	Pair	$D_{12}, \text{cm}^2/\text{s}$				
		$T = 273 \text{ K}$	$T = 298 \text{ K}$	$T = 323 \text{ K}$	$T = 348 \text{ K}$	$T = 373 \text{ K}$
1	$\text{CH}_4\text{--C}_2\text{H}_6$	0.150	0.175	0.201	0.230	0.259
2	$\text{CH}_4\text{--C}_3\text{H}_8$	0.099	0.115	0.132	0.151	0.170
3	$\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$	0.113	0.132	0.152	0.174	0.195
4	$\text{CH}_4\text{--CO}_2$	0.156	0.182	0.210	0.241	0.270
5	$\text{CO}_2\text{--N}_2$	0.192	0.224	0.258	0.295	0.332
6	$\text{CH}_4\text{--N}_2$	0.189	0.234	0.287	0.324	0.410
7	$\text{C}_3\text{H}_8\text{--N}_2$	0.096	0.119	0.146	0.176	0.207

The calculation using the Fuller method was performed based on the semi-empirical correlation:

$$D_{12}^{\text{Fuller}} = 0.00143 \frac{T^{1.75}}{p \left[(\Sigma V)_1^{1/3} + (\Sigma V)_2^{1/3} \right]^2} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}}, \quad (1)$$

where D_{12}^{Fuller} is the binary diffusion coefficient (cm^2/s), T is the temperature (K), p is the pressure (atm), M_1 and M_2 are the molar masses of the components, and ΣV_i is the diffusion volume of the i -th component, defined as the sum of atomic and structural contributions. The Fuller equation was derived based on the generalization of a large number of experimental data for dilute gases and represents an engineering method that provides acceptable accuracy (10–20%) without requiring knowledge of intermolecular interaction potentials [2, 5].

The Chapman–Enskog method is based on solving the Boltzmann kinetic equation for a dilute gas using the Lennard-Jones approximation for the intermolecular potential [1, 4]. In this case, the binary diffusion coefficient is expressed as follows:

$$D_{12}^{\text{CE}} = \frac{0.001858 T^{1.5} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}}}{p \sigma_{12}^2 \Omega_D(T^*)}, \quad (2)$$

where D_{12}^{CE} is the binary diffusion coefficient calculated using the Chapman–Enskog method; T is the absolute temperature; M_1 and M_2 are the molar masses of the two components; p is the pressure; σ_{12} is the effective Lennard-Jones collision diameter; $\Omega_D(T^*)$ is the diffusion collision integral; $T^* = kT/\varepsilon_{12}$ is the reduced temperature; k is the Boltzmann constant; and ε_{12} is the Lennard-Jones potential well depth for the interacting molecular pair [14, 15]:

$$\sigma_{12} = \frac{\sigma_1 + \sigma_2}{2}, \quad (3)$$

$$\varepsilon_{12} = \sqrt{\varepsilon_1 \varepsilon_2}. \quad (4)$$

The function $\Omega_D(T^*)$ was determined using approximations and linearly interpolated for intermediate values of T^* . The values of σ and ε/k for individual gases were taken from reference sources, ensuring reproducibility of the calculations and compatibility with modern thermodynamic models.

The comparison between theoretical and experimental values was carried out in dimensionless form using the relative deviation:

$$\Delta_i = \frac{D_{12}^{\text{model}} - D_{12}^{\text{exp}}}{D_{12}^{\text{exp}}} \times 100\%. \quad (5)$$

The accuracy analysis was performed separately for each temperature set, as well as averaged over all data points for each pair. To quantitatively assess the agreement between the models and experimental data, the mean absolute error (MAE) was used. These metrics made it possible not only to determine the average level of deviation but also to identify trends—systematic overestimation or underestimation of D_{12} for certain types of mixtures [12, 13, 22].

All calculations were carried out at a pressure of 1 atm, which eliminates the need to introduce compressibility corrections. The temperature range of 273–373 K ensures verification of the temperature sensitivity of the models within the region where the behavior of diffusion coefficients remains nearly linear in the coordinates D versus $T^{1.75}$ [10]. The adopted methodology allows for a rigorous validation of theoretical and semi-empirical models, as well as determination of their applicability limits for engineering calculations of systems containing hydrocarbon and non-hydrocarbon components.

3. RESULTS AND DISCUSSION

Based on the experimental data [3] and calculations performed using the Fuller and Chapman–Enskog equations, temperature dependencies of binary diffusion coefficients were obtained for seven binary gas systems at a pressure of 1 atm. All results are presented in Table 2 [3, 10, 14]. For each pair, the calculated values D_{12}^{Fuller} and D_{12}^{CE} were compared with the experimental values D_{12}^{exp} at temperatures of 273–373 K.

In all systems, a typical increase of D_{12} with temperature is observed, which corresponds to a power-law dependence $D \propto T^{1.75}$, characteristic of dilute gases. At the same time, temperature sensitivity varies depending on the type of components: mixtures of light gases ($\text{CH}_4\text{--N}_2$, $\text{CH}_4\text{--C}_2\text{H}_6$) exhibit a stronger increase in D upon heating than systems with heavier components ($\text{C}_2\text{H}_6\text{--C}_3\text{H}_8$, $\text{C}_3\text{H}_8\text{--N}_2$).

The comparison shows that the Chapman–Enskog (CE) method provides better results for most systems, ensuring an average relative error of less than $\pm 15\%$ over the entire temperature range. The Fuller method, in contrast, systematically overestimates diffusion coefficients, especially for mixtures containing heavy or asymmetric hydrocarbons, where the error reaches 30–70%.

For the $\text{CH}_4\text{--C}_2\text{H}_6$ and $\text{CH}_4\text{--C}_3\text{H}_8$ pairs, the Fuller calculation shows an overestimation of about 35–70% relative to experimental data. This is explained by the fact that the diffusion volumes used in the Fuller correlation were determined based on light nonpolar molecules and do not account for internal degrees of freedom and differences in molecular geometry of hydrocarbons [2, 14, 15]. At the same time, the Chapman–Enskog model, based on the Lennard–Jones potential, better reproduces experimental data (deviations do not exceed $\pm 10\%$), indicating an adequate consideration of differences in particle diameters and interaction energy.

Recent studies have proposed modified correlation-based and molecular-model approaches to improve the prediction of binary diffusion coefficients for complex gas mixtures. In particular, simplified

Table 2. Experimental and calculated binary diffusion coefficients of gas mixtures at 1 atm in the temperature range 273–373 K, calculated using the Fuller and Chapman–Enskog models [2, 4]

Gas pair	T , K	D_{exp} , cm ² /s	D_{Fuller} , cm ² /s	D_{CE} , cm ² /s	Δ_{Fuller} , %	Δ_{CE} , %
CH ₄ –C ₂ H ₆	273	0.150	0.204	0.138	+36%	–8%
	298	0.175	0.238	0.161	+36%	–8%
	323	0.201	0.274	0.187	+36%	–7%
	348	0.230	0.310	0.212	+35%	–8%
	373	0.259	0.352	0.239	+36%	–8%
CH ₄ –C ₃ H ₈	273	0.099	0.169	0.117	+71%	+18%
	298	0.115	0.197	0.136	+71%	+18%
	323	0.132	0.227	0.157	+72%	+19%
	348	0.151	0.259	0.177	+71%	+17%
	373	0.170	0.291	0.200	+71%	+18%
C ₂ H ₆ –C ₃ H ₈	273	0.113	0.120	0.085	+6%	–25%
	298	0.132	0.140	0.099	+6%	–25%
	323	0.152	0.162	0.114	+7%	–25%
	348	0.174	0.185	0.129	+6%	–26%
	373	0.195	0.208	0.147	+7%	–25%
CH ₄ –CO ₂	273	0.156	0.218	0.164	+40%	+5%
	298	0.182	0.254	0.190	+39%	+4%
	323	0.210	0.293	0.218	+39%	+4%
	348	0.241	0.334	0.248	+39%	+3%
	373	0.270	0.376	0.277	+39%	+3%
CO ₂ –N ₂	273	0.192	0.199	0.164	+4%	–15%
	298	0.224	0.232	0.191	+4%	–15%
	323	0.258	0.268	0.220	+4%	–15%
	348	0.295	0.305	0.251	+3%	–15%
	373	0.332	0.344	0.283	+4%	–15%
CH ₄ –N ₂	273	0.189	0.264	0.207	+40%	+10%
	298	0.234	0.308	0.242	+32%	+3%
	323	0.287	0.355	0.279	+24%	–3%
	348	0.324	0.405	0.316	+25%	–3%
	373	0.410	0.456	0.356	+11%	–13%
C ₃ H ₈ –N ₂	273	0.096	0.153	0.113	+59%	+18%
	298	0.119	0.178	0.131	+50%	+10%
	323	0.146	0.205	0.151	+41%	+3%
	348	0.176	0.234	0.172	+33%	–2%
	373	0.207	0.263	0.194	+27%	–6%

Lennard–Jones models, molecular-dynamics simulations, and data-driven correlations can reduce systematic deviations observed with conventional Fuller diffusion volumes by accounting more explicitly for molecular size, intermolecular interactions, and molecular structure [12, 13, 20, 22]. However, these approaches generally require additional molecular parameters or experimental calibration and therefore do not provide the same simplicity and universality as the original Fuller correlation.

The temperature dependence $D(T)$ for these pairs is close to a power law with an exponent of 1.7–1.8, which confirms kinetic-theory expectations.

For the C_2H_6 – C_3H_8 system, both methods show values close to experimental data, but Fuller slightly overestimates (by 6–7%), while Chapman–Enskog slightly underestimates (by 20–25%). This behavior is explained by the high similarity of molecular parameters of ethane and propane—their diffusion is mainly determined by mass differences and weak influence of interaction potentials. Since Fuller does not distinguish molecular shape, its error here is minimal. Thus, for structurally similar hydrocarbons, the Fuller method can be used with satisfactory accuracy.

In the CH_4 – CO_2 and CO_2 – N_2 systems, model deviations are smaller than in other cases. Fuller overestimates D by 4–40%, while CE shows deviations within $\pm 10\%$. For CO_2 – N_2 , the results of both methods practically coincide with experimental data, indicating the correctness of the chosen interaction potentials and the adequacy of the power-law relationship [16, 17, 18, 19, 20, 21].

Such good agreement is explained by the fact that CO_2 and N_2 have comparable Lennard–Jones diameters and similar interaction energy values, as well as low polarizability.

For CH_4 – N_2 and C_3H_8 – N_2 systems, opposite trends are observed. In the CH_4 – N_2 pair, Fuller overestimates D by about 30–40%, whereas Chapman–Enskog shows nearly perfect agreement at 298–323 K and moderate underestimation at higher temperatures. For C_3H_8 – N_2 , Fuller shows the typical overestimation of 25–50%, while CE demonstrates an accuracy of about $\pm 10\%$.

These results indicate that the influence of molecular mass and polarizability is significant: light gases (CH_4 , N_2) follow classical kinetic theory, whereas heavier and elongated molecules (C_3H_8) require accounting for anisotropic effects, which the Fuller method neglects.

For all seven systems, the mean absolute error (MAE) was: Fuller – 37% (range 6–70%); Chapman–Enskog – 11% (range 3–25%). The $D(T)$ plots show that the Chapman–Enskog curves almost coincide with the experimental points, whereas the Fuller curves systematically lie above them.

The discrepancy between the models increases with temperature, which is associated with different power-law dependences ($T^{1.75}$ and $T^{3/2}$): upon heating, the Fuller method responds more strongly than the actual experiment, leading to overestimation.

The difference in accuracy between the two methods has fundamental reasons. The Fuller model is correlation-based—it does not rely on microscopic physics but uses averaged diffusion volumes. In systems where molecules differ significantly in mass or geometry, this leads to an overestimation of the effective collision cross-section [14, 18, 19].

The Chapman–Enskog method, in contrast, is based on solving the Boltzmann equation and uses a realistic interaction potential (Lennard–Jones). Therefore, it more accurately describes diffusion as a function of mass, temperature, and molecular diameter.

The remaining deviations of the Chapman–Enskog model for hydrocarbon systems can be attributed to the limitations of the Lennard–Jones 12–6 potential, which assumes an effectively spherical and rigid molecular interaction. In polyatomic and chain-like hydrocarbons, part of the collision energy can be redistributed into internal rotational and vibrational modes, while molecular flexibility and anisotropic geometry lead to orientation-dependent interactions. As a result, not all collisions contribute equally to translational momentum transfer, which may reduce the effective collision efficiency and cause deviations from the diffusion coefficient predicted by the rigid 12–6 model [8, 9, 24].

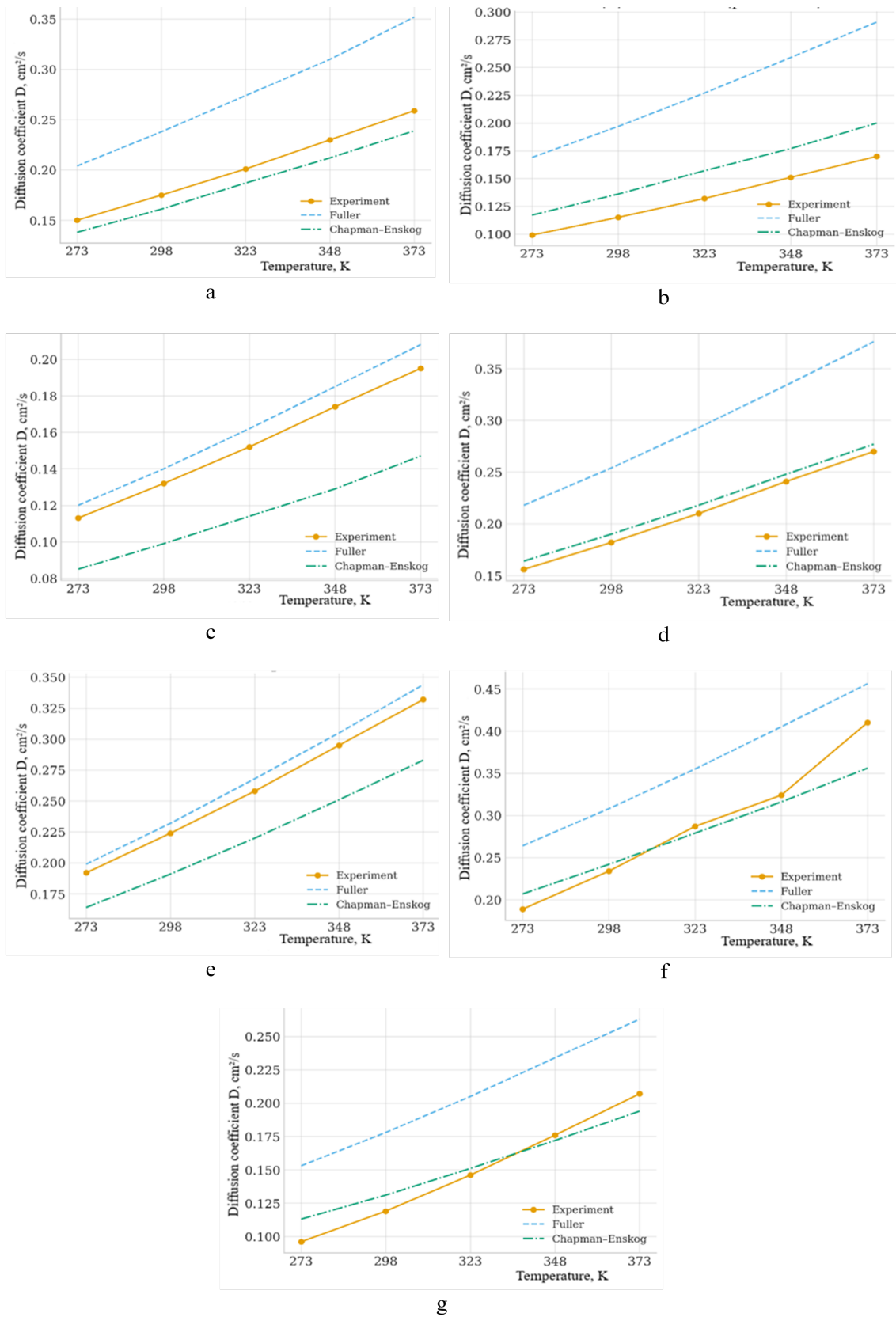


Figure 1 – Comparison of experimental and theoretical temperature dependences of the binary diffusion coefficient for gas mixtures: a) CH₄-C₂H₆; b) CH₄-C₃H₈; c) C₂H₆-C₃H₈; d) CH₄-CO₂; e) CO₂-N₂; f) CH₄-N₂; g) C₃H₈-N₂.

4. CONCLUSION

The conducted study made it possible to establish the patterns of variation in binary diffusion coefficients of gas mixtures of different compositions and nature in the temperature range of 273–373 K at atmospheric pressure. A systematic comparison of experimental data with calculations using the semi-empirical Fuller model and the kinetic-theory Chapman–Enskog equation showed that both approaches capture the general trend of diffusion increasing with temperature, but differ significantly in accuracy and physical interpretation.

The Fuller method, based on diffusion volume correlations, demonstrates a systematic overestimation of D_{12} , especially for mixtures containing heavy and asymmetric hydrocarbons. This is due to its limited ability to account for the fine structure of molecular interactions. At the same time, the Chapman–Enskog model, which employs the Lennard–Jones potential and a microscopic description of collisions, reproduces experimental values with high accuracy (average deviation does not exceed 10–15%) and correctly reflects the influence of molecular mass, size, and nature [2, 4, 14].

The obtained results are of particular importance for engineering and computational applications. The derived temperature dependences and accuracy assessment of the models can be used in mass transfer calculations for multicomponent mixtures, modeling of combustion, gas separation and mixing processes, as well as in numerical simulations. It is shown that the combination of experimental data and the Chapman–Enskog model provides a physically grounded and quantitatively reliable description of diffusion properties, making it the preferred choice for scientific and engineering tasks.

For example, in CFD modeling of gas mixing in a natural gas pipeline or combustion chamber, the binary diffusion coefficient directly affects the predicted rate of species mixing and the thickness of concentration boundary layers. Using a diffusion coefficient overestimated by 30–40% in a CFD model can potentially lead to an artificially accelerated mixing process, which, in turn, may result in inaccurate predictions of the local fuel–air mixture composition and, consequently, the characteristics of combustion and heat transfer. This effect is particularly important for hydrocarbon-rich mixtures, for which the Fuller correlation may substantially overestimate the diffusion coefficient.

Thus, the results not only confirm the applicability of classical kinetic theories but also provide a basis for further improvement of empirical correlations that account for complex intermolecular interactions in hydrocarbon and gas systems. The presented dependencies can serve as a benchmark for future numerical studies and the development of universal models for binary diffusion in polyatomic gas mixtures.

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DIFFUSIVE INSTABILITY AND CONCENTRATION CONVECTION IN A THREE-COMPONENT GAS SYSTEM $0.360\text{C}_3\text{H}_8 + 0.640\text{N}_2\text{O} - \text{CO}_2$

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Abstract. Isothermal mixing in multicomponent gas media is a strongly nonlinear process in which molecular transport may give way to solutal gravitational convection, changing the intensity of mass transfer substantially. This transition is investigated using the system $0.360\text{C}_3\text{H}_8 + 0.640\text{N}_2\text{O} - \text{CO}_2$, in which the molar masses of all components differ by less than 0.2%, so that stratification driven by molecular-weight differences is excluded and the role of diffusive instability can be isolated. Three-dimensional unsteady modelling was performed with the Species Transport formulation (ANSYS Fluent) and compared with two-flask experimental data over the pressure range 0.2–0.85 MPa at $T = 298$ K. The agreement is characterised by a mean absolute error of 0.0106 mole fraction, a root-mean-square error of 0.0109, a mean absolute percentage error of 9.1% and a mean signed relative deviation of -1.3% , the last indicating the absence of systematic bias. It is shown that the upper mixture is denser than the underlying carbon dioxide over the entire pressure range examined, the relative density excess growing from about 1.0% at 0.2 MPa to about 6.0% at 1.0 MPa; this excess originates entirely from the difference in compressibility factors rather than from molar masses, and is confirmed by an independent Peng–Robinson calculation. Convection therefore sets in not through a change in the sign of the density difference but through the Rayleigh number crossing its critical range, which occurs between 0.3 and 0.4 MPa and coincides with the steep experimental rise of propane transport.

Keywords: multicomponent gas mixture; diffusive instability; solutal gravitational convection; density excess; Rayleigh number; Peng–Robinson equation of state; CFD modelling; ANSYS Fluent; mass transfer.

1. INTRODUCTION

Among the diverse types of motion in liquid and gaseous media, a special place is held by convection driven by the instability of the mechanical equilibrium of a mixture [1, 2]. Practical interest in this phenomenon stems from a wide range of applications, spanning gas separation, combined heat and mass transfer in chemical reactors, and atmospheric phenomena [3, 4]. In multicomponent media the situation becomes considerably more complex: differences in the mutual diffusion coefficients of the components give rise to strongly nonlinear concentration distributions, which alter the expected rate of composition homogenisation [5, 6].

A fundamental feature of multicomponent systems is that convective motion arises in them not only under the conditions of the classical Rayleigh–Bénard scheme [1, 2] but also in the presence of initially stable stratification, where the mixture density decreases with height. In this case the instability is governed by the relationship between several concentration gradients, and convective mass transport can exceed diffusive and thermodiffusive contributions by an order of magnitude or more [7]. Methodologies for predicting instability zones have been proposed to support accurate analysis [8, 9, 10].

Under isothermal conditions, effects associated with the diffusive mobility of the components, the pressure and the mixture composition become apparent. A review [11] and a number of experimental and theoretical studies [12, 13, 14] have shown that convective flows can arise in isothermal

multicomponent gas mixtures as early as the initial stage of mixing; moreover, under certain conditions preferential transport of the component with the highest molecular mass is observed. It has been established that the transition between regimes is determined not only by differences in diffusion coefficients but also by pressure and initial composition [15, 16, 17].

At the same time, the boundary between the diffusion and convection regimes in multicomponent gas mixtures has not been sufficiently studied. The case in which the component densities are close to one another remains virtually unexplored; here the stratification mechanism driven by differences in molecular masses is absent, and instability can arise solely from differences in diffusion fluxes and from deviations from ideal-gas behaviour. The $\text{C}_3\text{H}_8\text{--N}_2\text{O--CO}_2$ system is a convenient model for this type of study: the molar masses of its components differ by less than 0.2%, whereas their compressibility factors diverge significantly at the same pressure.

The aim of this study is to determine the mechanism of the transition from molecular diffusion to solutal gravitational convection in a system whose component molar masses differ by less than 0.2%, using the $0.360\text{C}_3\text{H}_8 + 0.640\text{N}_2\text{O} - \text{CO}_2$ composition as an example. The objectives are to perform three-dimensional unsteady modelling of mass transfer within the geometry of an actual two-flask apparatus, to verify the calculations against experimental data [18] over the range 0.2–0.85 MPa, to quantify the density excess and the corresponding Rayleigh number, and on this basis to explain the non-monotonic pressure dependence of mass transfer.

2. MATERIALS AND METHODS

2.1. Problem statement and experimental basis

The experimental data used to verify the calculations were obtained by the two-flask method [18]; a schematic of the setup is shown in Figure 1. Initially the internal volumes of the rig—the upper flask (1), the lower flask (2) and the connecting channel (3)—were evacuated with the shut-off valve (4) closed. The upper flask was then filled with a binary mixture of propane and nitrous oxide from cylinder (5) through valve (9), the pressure being adjusted to the experimental value and monitored with gauge (7). Similarly, the lower flask was filled with carbon dioxide from cylinder (6) through valve (10), with the pressure monitored by gauge (8). After the pressures in the flasks had equalised, valve (4) was opened and mixing began, with simultaneous recording of the time. After the set interval the channel was closed and the actual mixing time recorded; samples were withdrawn through valves (12) and (13) and analysed chromatographically (14).

Concentrations were determined by gas chromatography with an uncertainty of no more than 3%. Direct measurements were performed for propane and nitrous oxide, whereas the carbon dioxide concentration was derived from the condition of particle number conservation:

$$\sum_{i=1}^3 c_i = 1, \quad (1)$$

where c_i is the concentration of the i -th component. To improve reliability, the results were averaged over several series of measurements performed under identical conditions. In all experiments the upper flask contained the binary mixture of propane and nitrous oxide, while the lower flask contained carbon dioxide.

The geometric parameters of the cell were as follows: the volumes of the upper and lower flasks were $226.8 \cdot 10^{-6}$ and $214.5 \cdot 10^{-6} \text{ m}^3$ respectively; the connecting channel was a narrow slit with a cross-section of $0.005 \times 0.0006 \text{ m}^2$ and a height of $17 \cdot 10^{-3} \text{ m}$. The temperature was maintained constant at $T = 298 \text{ K}$ in all experiments, so that the system was strictly isothermal; the duration of

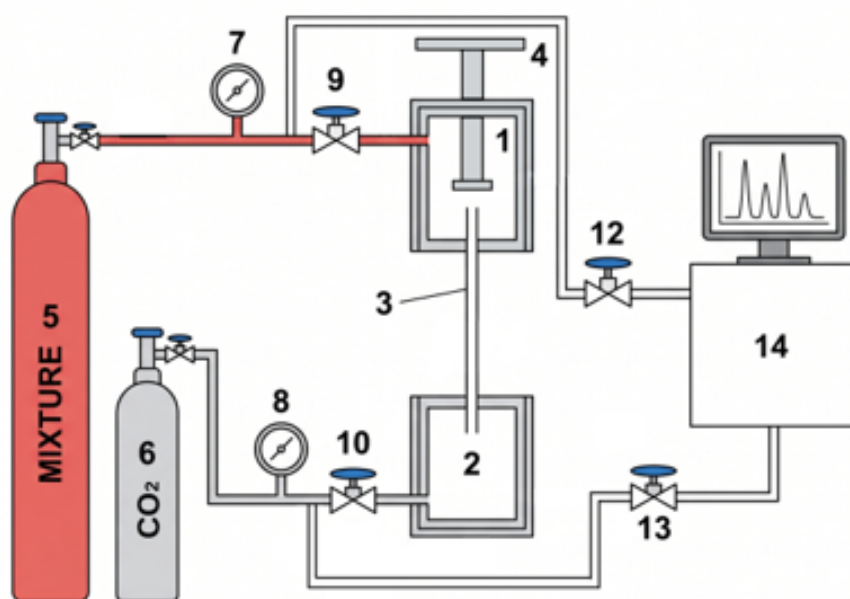


Figure 1 – Schematic of the experimental setup

each experiment was 20 min. The present study examines a single initial composition of the upper mixture, $0.360\text{C}_3\text{H}_8 + 0.640\text{N}_2\text{O}$, which makes it possible to follow the entire sequence of regimes on one object without averaging across compositions.

2.2. Thermophysical characteristics of the components

The input data for the calculation—density ρ , dynamic viscosity η and compressibility factor Z of the components at $T = 298\text{ K}$ —are listed in Table 1 from reference sources [19, 20].

Table 1. Density and compressibility factor of the components at $T = 298\text{ K}$ [19, 20]

p, MPa	$\rho(\text{C}_3\text{H}_8), \text{kg/m}^3$	$\rho(\text{N}_2\text{O}), \text{kg/m}^3$	$\rho(\text{CO}_2), \text{kg/m}^3$	$Z(\text{C}_3\text{H}_8)$	$Z(\text{N}_2\text{O})$	$Z(\text{CO}_2)$
0.2	3.74	3.65	3.64	0.966	0.988	0.989
0.3	5.64	5.52	5.50	0.948	0.981	0.983
0.4	7.58	7.42	7.38	0.929	0.974	0.977
0.5	9.56	9.36	9.29	0.910	0.966	0.970
0.6	11.60	11.35	11.23	0.890	0.958	0.963
0.7	13.70	13.39	13.21	0.870	0.950	0.956
0.8	15.87	15.48	15.23	0.849	0.942	0.949
0.9	18.12	17.63	17.29	0.827	0.933	0.941
1.0	20.46	19.84	19.40	0.804	0.924	0.933

The molar masses of the components are close to one another: $M(\text{C}_3\text{H}_8) = 44.097 \cdot 10^{-3}$, $M(\text{N}_2\text{O}) = 44.013 \cdot 10^{-3}$ and $M(\text{CO}_2) = 44.009 \cdot 10^{-3}\text{ kg/mol}$. The dynamic viscosity varies only slightly within the pressure range considered— $\eta(\text{C}_3\text{H}_8) = 8.31\text{--}8.62$, $\eta(\text{N}_2\text{O}) = 14.93\text{--}15.17$ and $\eta(\text{CO}_2) = 15.02\text{--}15.26$ (in units of $10^{-6}\text{ N} \cdot \text{s/m}^2$)—in agreement with the kinetic theory of gases, according to which the viscosity of a rarefied gas is determined primarily by temperature. The compressibility factors, in contrast, differ significantly: at 1.0 MPa , $Z(\text{C}_3\text{H}_8) = 0.804$ whereas $Z(\text{CO}_2) = 0.933$. It is this dis-

crepancy, rather than the difference in molar masses, that governs the formation of the density excess (Section 4.1).

The mutual diffusion coefficients of the components [19, 20] decrease with increasing pressure according to $D \propto 1/p$, reflecting the reduction of the molecular mean free path as the gas is compressed. At $p = 0.2$ MPa they are $D(\text{C}_3\text{H}_8\text{--CO}_2) = 0.218 \cdot 10^{-5}$, $D(\text{C}_3\text{H}_8\text{--N}_2\text{O}) = 0.215 \cdot 10^{-5}$ and $D(\text{CO}_2\text{--N}_2\text{O}) = 0.298 \cdot 10^{-5} \text{ m}^2/\text{s}$, and at $p = 0.5$ MPa $0.087 \cdot 10^{-5}$, $0.086 \cdot 10^{-5}$ and $0.119 \cdot 10^{-5} \text{ m}^2/\text{s}$ respectively. Two features of this data set are relevant to what follows. First, the $\text{CO}_2\text{--N}_2\text{O}$ pair diffuses faster than either pair involving propane, the ratio $D(\text{CO}_2\text{--N}_2\text{O})/D(\text{C}_3\text{H}_8\text{--CO}_2)$ remaining close to 1.37 over the whole pressure range; this asymmetry of diffusive mobilities creates local non-equilibrium density distributions in the transition zone of the channel, which act as the initial perturbation for the instability. Second, the two binary coefficients that involve propane differ from one another by only 0.9–2.3%, a point returned to in Section 4.4.

2.3. Computational domain and mesh generation

The problem was solved in a three-dimensional formulation: only a 3D model permits an accurate description of spatially non-uniform concentration fields, the formation of convective cells, and possible flow asymmetry in the region of the connecting channel. The computational domain reproduced the geometry of the actual two-flask apparatus (Figure 2).

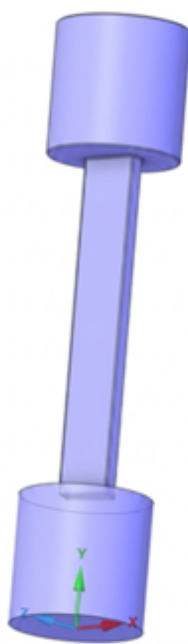


Figure 2 – Three-dimensional model of the two-flask diffusion cell

Discretisation was performed on a three-dimensional unstructured tetrahedral mesh with local refinement in the diffusion channel and in the adjacent parts of the flasks, where the concentration and velocity gradients are largest and where the first signs of instability appear. The element size in the bulk volumes of the flasks was $1.5 \cdot 10^{-3} \text{ m}$, while a refined size of 10^{-4} m was used in the connecting channel. The total number of cells in the computational domain was 1,038,742. The refinement level in the channel was selected so that its narrowest transverse dimension ($0.6 \cdot 10^{-3} \text{ m}$) was resolved by six cells across, which is the minimum required to represent the transverse velocity profile of the developing exchange flow. A formal grid-convergence study is discussed in Section 4.4.

2.4. Physical models and governing equations

Modelling was performed in a transient three-dimensional formulation using the Species Transport module of ANSYS Fluent. Mass transport was treated as a coupled process involving molecular diffusion and transport driven by the motion of the mixture as a whole. The mass conservation equation for each species was written in integral form for an arbitrary control volume V bounded by a surface S :

$$\frac{d}{dt} \int_V \rho Y_i dV + \int_S \rho Y_i \mathbf{v} \cdot d\mathbf{S} = - \int_S \mathbf{j}_i \cdot d\mathbf{S}, \quad (2)$$

where Y_i is the mass fraction of the i -th component, ρ is the mixture density, $\mathbf{v}$ is the velocity vector and $\mathbf{j}_i$ is the diffusion flux. This form directly expresses the mass balance within each cell and is convenient for the finite-volume implementation [22].

The hydrodynamic behaviour of the mixture was described by the momentum conservation equations, with the density treated as a function of the local composition. The concentration and velocity fields are therefore coupled; redistribution of the components alters the density, which in turn influences the flow structure. This feedback constitutes the physical basis of solutal gravitational convection.

The SST $k-\omega$ model [23] was employed for closure. The convective velocities developing in the connecting channel are small and the flow remains laminar throughout the process, so that the turbulent viscosity produced by the model is negligible relative to the molecular viscosity and the formulation reduces in practice to a laminar one. The model was retained for robustness in the presence of steep gradients within the confined channel geometry; the associated limitation is discussed in Section 4.4.

Binary mutual diffusion coefficients were determined from the kinetic theory of gases using Chapman–Enskog-type relations [24]:

$$D_{ij} \sim \frac{T^{3/2}}{p \sigma_{ij}^2 \Omega_{ij}}, \quad (3)$$

where σ_{ij} is the effective collision diameter, Ω_{ij} the collision integral, T the temperature and p the pressure. This relation accounts for the decrease of D_{ij} with pressure noted in Section 2.2.

2.5. Numerical solution procedure

The choice of numerical schemes was dictated by the need to describe unsteady mass transfer accurately in the presence of pronounced concentration gradients while minimising numerical diffusion, which could distort the transport characteristics within the channel. A second-order approximation was used for the momentum and turbulence transport equations in order to improve the representation of velocity and concentration gradients, which is critical when analysing the transition between regimes [21]. The PRESTO! scheme was used for pressure, ensuring a correct pressure distribution in problems involving gravitational effects; gradients were evaluated by the least-squares method, which improves stability on unstructured meshes. The nonlinear system was solved iteratively, the velocity, pressure and concentration fields being refined successively at each time step until convergence.

3. RESULTS

3.1. Pressure dependence of propane transport

The mole fraction of propane in the lower flask was selected as the representative parameter characterising the intensity of inter-flask mass transfer. This choice follows from the fact that the

component concentrations of a ternary system are linked by the material balance condition (1), so that analysing the remaining components yields no fundamentally new information. A comparison of the calculated results with the experimental data [18] is presented in Table 2.

Table 2. Mole fraction of propane in the lower flask for the composition $0.360 \text{ C}_3\text{H}_8 + 0.640 \text{ N}_2\text{O} - \text{CO}_2$

p , MPa	Experiment [18]	ANSYS Fluent
0.20	0.092	0.086
0.30	0.105	0.118
0.45	0.138	0.127
0.55	0.140	0.150
0.85	0.115	0.102

The agreement was assessed using several complementary measures, since a single figure of merit can be misleading for a data set of this size. The mean absolute error is 0.0106 and the root-mean-square error 0.0109 mole fraction; in relative terms the mean absolute percentage error is 9.1% and the largest single deviation 12.4%. These quantities characterise the magnitude of the scatter. Its direction is characterised separately by the mean signed relative deviation, which amounts to only -1.3% ; the residuals alternate in sign and very nearly cancel, so that the model exhibits no systematic bias with respect to the experiment and the discrepancies are random in character. In absolute terms the residuals lie between 0.006 and 0.013 mole fraction. For comparison, the 3% uncertainty of the chromatographic determination corresponds to 0.003–0.004 mole fraction at the concentration levels considered, that is, roughly one third of the observed residual; the remainder is attributable to the model and to discretisation.

The largest relative deviation occurs at 0.30 MPa, that is, precisely at the regime-transition boundary identified in Section 4.2, where the system is most sensitive to initial perturbations and where the predicted onset of instability depends most strongly on the mesh resolution in the zone of maximum gradients. Outside the vicinity of this boundary, the agreement is noticeably better. Significantly, the model reproduces not only the absolute values but also the qualitative structure of the pressure dependence: propane transport increases with pressure, reaches a maximum at $p \approx 0.55$ MPa (0.140 in the experiment against 0.150 in the calculation) and then decreases, falling to 0.115 at 0.85 MPa. The non-monotonic character of the dependence is reproduced without any additional tuning of the model, which indicates that its origin is physical rather than numerical.

3.2. Time evolution of the propane concentration

The evolution of the propane mole fraction in the lower flask at $p = 0.583$ MPa, corresponding to the region of maximum transfer, is shown in Figure 3.

The curve divides clearly into three sections. In the initial interval ($t \lesssim 100$ s) the concentration rises rapidly to about 0.05, corresponding to the establishment of the diffusive flux immediately after the channel is opened. Subsequently, over $t \approx 100$ –400 s, the rate of increase falls noticeably and the dependence becomes quasi-diffusive; the concentration grows smoothly, without pronounced nonlinearities.

A qualitative change occurs over $t \approx 400$ –700 s. The rate of increase rises again and appreciably exceeds the values characteristic of the preceding quasi-diffusive stage, the concentration growing from ≈ 0.07 to ≈ 0.125 . Such an acceleration of transport under unchanged external conditions cannot be explained within a purely diffusive framework and indicates the onset of convective motion

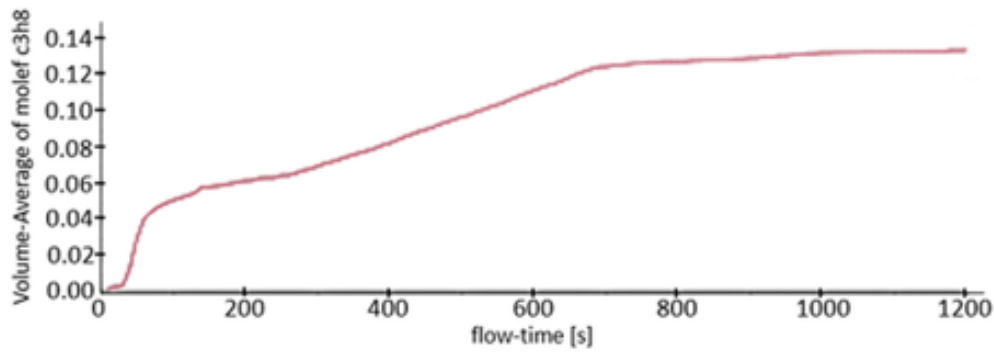


Figure 3 – Time evolution of the volume-averaged mole fraction of propane in the lower flask for the composition $0.360\text{C}_3\text{H}_8 + 0.640\text{N}_2\text{O} - \text{CO}_2$ at $p = 0.583\text{ MPa}$

in the channel. The interval $t^* \approx 400\text{--}600\text{ s}$ should be regarded as the delay time for the development of the instability, that is, the period required for the diffusive redistribution of the components to generate a sufficient density excess in the transition zone.

After $t \approx 700\text{ s}$ the curve enters a quasi-stationary regime, rising slowly to 0.135 by $t = 1200\text{ s}$. This saturation reflects the depletion of the driving concentration difference between the flasks as the compositions equalise.

4. DISCUSSION

4.1. Density excess as the source of the instability

The molar mass of the upper mixture, calculated from its initial composition, is $M = 0.360 \cdot 44.097 + 0.640 \cdot 44.013 = 44.043 \cdot 10^{-3}\text{ kg/mol}$, exceeding that of carbon dioxide by only 0.078% [cite: 9]. Under strict adherence to the ideal-gas equation of state such a difference would produce a relative density excess of the same order, a value far too small to drive convection in a channel of the dimensions considered. The instability mechanism must therefore be sought in the departure of the gases from ideality.

Writing the density of a real gas as $\rho = pM/(ZRT)$ and applying the additive rule $Z_{\text{mix}} = \sum x_i Z_i$ to the upper mixture, the relative density excess with respect to pure carbon dioxide at the same pressure and temperature takes the compact form:

$$\frac{\Delta\rho}{\rho} = \frac{\rho_{\text{mix}} - \rho_{\text{CO}_2}}{\rho_{\text{CO}_2}} = \frac{M_{\text{mix}}}{M_{\text{CO}_2}} \cdot \frac{Z_{\text{CO}_2}}{Z_{\text{mix}}} - 1. \quad (4)$$

Written in this form the result is immediate. Both factors exceed unity at every pressure: $M_{\text{mix}} > M_{\text{CO}_2}$ by construction, and $Z_{\text{mix}} < Z_{\text{CO}_2}$ because propane is markedly less ideal than carbon dioxide. The density excess is therefore positive throughout the pressure range, and no change of sign occurs. Its magnitude, however, is strongly pressure dependent, since the ratio $Z_{\text{CO}_2}/Z_{\text{mix}}$ grows as the gases are compressed. The computed values are given in Table 3.

Because the density excess is central to the proposed mechanism, the additive- Z approximation was verified independently against the Peng–Robinson equation of state with van der Waals mixing rules and zero binary interaction parameters, using standard critical constants for the three gases [26, 27]. This route gives a density excess that is likewise positive at every pressure, growing from +0.81% at 0.2 MPa to +2.02% at 0.5 MPa and +4.40% at 1.0 MPa. The two calculations therefore agree on every essential point: the sign of the excess, its monotonic growth with pressure, and its order of magnitude. The additive rule overestimates the excess by 0.2–1.6 percentage points, the

Table 3. Relative density excess of the upper mixture over carbon dioxide at $T = 298$ K

p , MPa	Z_{mix}	ρ_{mix} , kg/m ³	$\Delta\rho/\rho$, %
0.2	0.980	3.627	+0.99
0.3	0.969	5.503	+1.51
0.4	0.958	7.424	+2.08
0.5	0.946	9.397	+2.63
0.6	0.934	11.425	+3.24
0.7	0.921	13.507	+3.86
0.8	0.909	15.653	+4.53
0.9	0.895	17.878	+5.24
1.0	0.881	20.181	+6.01

discrepancy increasing with pressure as the mixture departs further from ideality—the expected behaviour, since additivity of compressibility factors is an Amagat-type approximation that neglects cross-interaction between unlike molecules. For the purposes of the present analysis this level of agreement is sufficient, and the conclusions drawn below are unchanged if the Peng–Robinson values are used instead.

The physical origin of the effect is the following. All three components have almost identical molar masses, so that under ideal behaviour their densities at a given pressure would coincide to within 0.08% at any pressure. In reality the density is governed by the ratio M/Z , and the behaviour of the compressibility factor becomes decisive. Of the gases considered, propane lies closest to its condensation region (the saturation pressure is about 0.9 MPa at 298 K), and its compressibility factor therefore falls much more rapidly with pressure—from 0.966 at 0.2 MPa to 0.804 at 1.0 MPa—whereas for carbon dioxide it falls only from 0.989 to 0.933[cite: 9]. A decrease in Z corresponds to an increase in density at the same pressure, so the presence of 36% propane in the upper flask makes that mixture heavier than pure CO₂, and increasingly so as the pressure rises. It is the non-ideality of propane, and not any difference in molecular masses, that maintains the heavy-over-light configuration.

A positive density excess is a necessary but not a sufficient condition for convection. The configuration is potentially unstable at every pressure examined, yet the experiment shows only weak transport at 0.2 MPa and a steep rise thereafter. The selection of the actual transition therefore rests with the balance between the destabilising buoyancy and the stabilising action of viscosity and diffusion, which is quantified by the Rayleigh number in the next section.

4.2. Rayleigh number

The stability of the configuration is characterised by the solutal Rayleigh number

$$\text{Ra} = \frac{g \left(\frac{\Delta\rho}{\rho} \right) L^3}{\nu D}, \quad \nu = \frac{\eta_{\text{mix}}}{\rho_{\text{mix}}}, \quad (5)$$

in which the choice of the characteristic length L requires comment, since the connecting channel has two very different transverse dimensions and a third, much larger, longitudinal one. Two scales are physically meaningful. The channel height $H = 17 \cdot 10^{-3}$ m is the distance over which the density difference between the flasks is supported and therefore sets the total buoyant driving force available to the exchange flow. The narrower transverse dimension of the slit, $d = 0.6 \cdot 10^{-3}$ m, is the scale that controls the onset of the instability, because it limits the size of the disturbance that can develop across the channel and it is over this distance that viscous damping acts. Rayleigh numbers based on the two

scales differ by the factor $(H/d)^3 \approx 2.3 \cdot 10^4$ and must be compared with different critical values. The kinematic viscosity was evaluated as $\nu = \eta/\rho$, the mixture viscosity $\eta \approx 12.5 \cdot 10^{-6} \text{ N} \cdot \text{s}/\text{m}^2$ being obtained from the additive rule, and D was taken as the $\text{C}_3\text{H}_8\text{--CO}_2$ coefficient at the corresponding pressure (Section 2.2).

Evaluated on the channel height, Ra grows from $6.3 \cdot 10^4$ at 0.2 MPa to $1.1 \cdot 10^6$ at 0.5 MPa and $1.1 \cdot 10^7$ at 1.0 MPa. Evaluated on the slit width, which is the scale relevant to the onset of the disturbance, it grows from 2.8 at 0.2 MPa to 9.7 at 0.3 MPa, 24 at 0.4 MPa and 48 at 0.5 MPa, reaching $4.7 \cdot 10^2$ at 1.0 MPa. This growth is driven by the combined effect of an increasing density excess and a diffusion coefficient falling as $1/p$. Since the product $\rho\nu = \eta$ is practically independent of pressure, equation (5) implies the approximate relation $Ra \propto (\Delta\rho/\rho) \cdot p$, which accounts for the roughly quadratic growth with pressure.

The essential point is that the Rayleigh number based on the slit width passes through values of order 10 between 0.3 and 0.4 MPa. For confined vertical geometries with an axial density gradient the critical Rayleigh number is of order $10^1\text{--}10^2$ depending on the aspect ratio and the boundary conditions [1, 2], so this crossing brackets precisely the interval over which the measured propane transport rises steeply, from 0.105 at 0.30 MPa to 0.138 at 0.45 MPa (Table 2). The transition observed in the experiment is therefore identified with the crossing of the critical Rayleigh number rather than with any change in the sign of the density difference. It should be emphasised that a critical value specific to the present slit geometry would require a dedicated linear stability analysis, which lies outside the scope of this work; the comparison made here is an order-of-magnitude one. Independent estimates of the convective velocity in the channel confirm that the resulting flow remains laminar over the whole range of conditions examined.

4.3. Nature of the pressure maximum

The monotonic growth of the Rayleigh number apparently contradicts the transport maximum observed in Table 2 at $p \approx 0.55$ MPa. The contradiction is removed once it is recognised that the measured quantity is a mole fraction and not an absolute mass flux. At fixed volume the total number of moles of gas in the lower flask increases in proportion to the pressure, so that even for a rising absolute flux of propane the mole fraction, normalised by this total, can pass through a maximum. The pressure maximum thus reflects the competition between the intensification of convective transport, driven by the increase of Ra , and the simultaneous dilution of the transported material within an increasing total number of particles.

A second factor is hydrodynamic. As the pressure rises, the diffusion coefficient continues to fall as $1/p$ while the convective velocity grows, and the exchange flow in a slit of high aspect ratio may reorganise from a through-going counter-flow into a system of closed recirculation cells localised within the channel. Such cells would mix the fluid efficiently inside the channel while contributing little to the net inter-flask transport, so that the overall transfer would again become diffusion-limited. This interpretation is consistent with observations reported for related two-flask systems at elevated pressures [13, 17], but it is offered here as a hypothesis: the present calculations were post-processed for concentration fields only, and a dedicated analysis of velocity vectors and streamlines at several pressures would be required to establish the existence and the geometry of such cells directly. This is identified as the principal direction for the continuation of the work.

4.4. Model limitations

Several limitations of the present approach should be borne in mind when interpreting the results. Diffusive transport was described through effective binary coefficients, whereas a rigorous treat-

ment of a ternary system requires the full Maxwell–Stefan matrix [25]. The magnitude of this simplification can be bounded from the data of Section 2.2. The species that carries the density signal is propane, and its two binary coefficients, $D(\text{C}_3\text{H}_8\text{--CO}_2)$ and $D(\text{C}_3\text{H}_8\text{--N}_2\text{O})$, differ from each other by only 0.9–2.3% across the entire pressure range. The effective diffusivity of propane is therefore almost independent of the local ratio of CO_2 to N_2O in the surrounding medium, and the binary approximation is well justified for the component that governs the buoyancy. The substantial difference in mobilities, a factor of 1.37, is between CO_2 and N_2O , that is, within the pair that does not carry a significant density contrast. Cross-diffusion effects are consequently expected to redistribute these two components relative to one another rather than to alter the propane flux appreciably; their neglect is not expected to change the conclusions, although it may shift the predicted onset time.

The mutual diffusion coefficients were held constant throughout the computational domain and were not adjusted for the local composition, whereas in the transition zone of the channel the composition varies over a wide range. Including the concentration dependence of D_{ij} would refine the predicted onset of convection.

The SST $k\text{--}\omega$ closure was applied to a flow which remains laminar over the whole range of conditions examined. The turbulent viscosity generated by the model is small compared with the molecular value, so the computation is effectively laminar; nevertheless a residual eddy viscosity cannot be excluded near the sharp gradients at the channel entrance, where it would act as an additional effective diffusivity and could shift the calculated onset time. A direct comparison with a fully laminar computation at two or three representative pressures is planned and will quantify this effect.

Finally, the mesh was refined locally in the channel to the level described in Section 2.3 rather than through a formal grid-convergence study on a sequence of systematically refined meshes. Because the predicted onset time of the instability is the quantity most sensitive to resolution, a study of this kind—reporting both the final concentration and the onset time as functions of cell count—is required to establish the numerical uncertainty of the present results and is the subject of ongoing work.

5. CONCLUSION

An experimental and numerical study of isothermal mixing in a three-component gas system has been carried out for the composition $0.360 \text{ C}_3\text{H}_8 + 0.640 \text{ N}_2\text{O} - \text{CO}_2$ over the pressure range 0.2–0.85 MPa at a constant temperature of $T = 298 \text{ K}$. The main results are as follows:

1. A three-dimensional CFD model based on the Species Transport approach reproduces the propane mole fraction in the lower flask with a mean absolute error of 0.0106 mole fraction, a root-mean-square error of 0.0109 and a mean absolute percentage error of 9.1%, the maximum relative deviation being 12.4%. The mean signed relative deviation of -1.3% shows that the model carries no systematic bias. The largest deviation occurs at the regime-transition boundary, where the predicted onset of instability is most sensitive to mesh resolution. The model reproduces the non-monotonic pressure dependence with a maximum at $p \approx 0.55 \text{ MPa}$.
2. In a system whose component molar masses differ by less than 0.2%, the upper mixture is nevertheless denser than the underlying carbon dioxide at every pressure examined, the relative density excess growing from about 1.0% at 0.2 MPa to about 6.0% at 1.0 MPa. The excess arises entirely from the difference in compressibility factors—propane, being closest to its condensation region, departs from ideality far more strongly than carbon dioxide—and not from the difference in molar masses, which would account for only 0.08%. An independent Peng–Robinson calculation confirms the sign, the monotonic growth and the order of magnitude of this excess.
3. Since the density excess is positive throughout, the onset of convection is not governed by a

change in the sign of the density difference but by the Rayleigh number crossing its critical range. Evaluated on the slit width, Ra grows from 2.8 at 0.2 MPa to 48 at 0.5 MPa and passes through values of order 10 between 0.3 and 0.4 MPa, that is, precisely over the interval in which the measured transport rises steeply.

4. The time evolution of the concentration exhibits three characteristic stages—an initial diffusive stage, a quasi-diffusive stage and a convective stage—with a delay time for the development of the instability of $t^* \approx 400\text{--}600$ s, after which the transport rate increases markedly.
5. The non-monotonic pressure dependence is explained by the competition between the intensification of convective transport, which follows the growth of the Rayleigh number, and the dilution of the transported material within the total number of particles, which increases with pressure.

The results obtained may serve as a basis for formulating quantitative criteria for identifying mixing regimes in multicomponent gas systems with a negligible initial molar-mass contrast, and for selecting conditions for the accurate measurement of mutual diffusion coefficients, whose reliable determination is possible only in the strictly diffusive regime.

AUTHOR CONTRIBUTIONS

V. Mukamedenkyzy — conceptualisation, methodology, supervision, manuscript editing; B.E. Akberdiyev — numerical modelling, data processing and analysis, visualisation, preparation of the initial draft; N.G. Valko — analysis of results, methodological review, manuscript editing. All authors have read and approved the final version of the manuscript.

DATA AVAILABILITY

Data supporting the results of this study are available from the corresponding author upon reasonable request. Experimental data used for verification were taken from previously published work.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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BOSON MAPPINGS OF THE FERMION DYNAMICAL SYMMETRY MODEL AND STRUCTURAL EVOLUTION OF $^{186-192}\text{Os}$

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Abstract. This work examines the microscopic connection between the fermion dynamical symmetry model (FDSM) and an effective bosonic description of collective nuclear states. A simplified FDSM Hamiltonian containing monopole and quadrupole pairing terms together with proton and neutron multipole interactions is mapped onto an s - d boson space by three procedures: the generalized Dyson mapping, a seniority-based Hermitization, and the Belyaev–Zelevinsky expansion. The role of the physical boson subspace, Hermiticity, and the truncation of the boson expansion to one- and two-body operators is discussed. The Dyson representation preserves the fermionic matrix elements in the appropriate physical subspace but is generally non-Hermitian in the conventional boson metric. The seniority and Belyaev–Zelevinsky procedures provide Hermitian IBM-like Hamiltonians that can be compared directly with the interacting boson model. The mapped Hamiltonians are applied to the even osmium isotopes ^{186}Os , ^{188}Os , ^{190}Os , and ^{192}Os . The effective parameters evolve comparatively smoothly from ^{186}Os to ^{190}Os , whereas several coefficients show a pronounced rearrangement at ^{192}Os . The same mass region is singled out by different mappings, supporting an interpretation in terms of a change in the effective collective structure. The parameter discontinuity alone is not taken as proof of a quantum phase transition; further tests using spectra, $B(E2)$ values, quadrupole observables, and collective energy surfaces are required.

Keywords: Fermion dynamical symmetry model; interacting boson model; boson mapping; Dyson mapping; seniority; Belyaev–Zelevinsky mapping; collective nuclear structure; osmium isotopes.

1. INTRODUCTION

Collective excitations in medium-mass and heavy nuclei provide a characteristic example of emergent behavior in a finite quantum many-body system. Low-lying states of even-even nuclei often display vibrational, rotational, or transitional regularities although the underlying degrees of freedom are interacting protons and neutrons. A direct shell-model description becomes increasingly difficult as the valence space grows, and this has motivated collective truncation schemes in which the dominant correlated degrees of freedom are treated explicitly [1, 2, 3, 4, 5, 6, 7]

The interacting boson model (IBM) is one of the most successful algebraic descriptions of such collective motion. Its basic degrees of freedom are s and d bosons with angular momenta $L = 0$ and $L = 2$. The dynamical limits of the model reproduce broad classes of collective spectra, while the Otsuka–Arima–Iachello construction provides a microscopic interpretation of the bosons as correlated nucleon pairs [1, 2, 3, 4, 5]. This microscopic connection is important because it allows the parameters of an effective boson Hamiltonian to be related, at least in principle, to the structure of a fermionic valence space.

Pairing and seniority provide a natural bridge between shell-model and boson descriptions. When low-lying states are dominated by coherent pairs, a large fermion space can be reduced to a much smaller subspace containing a limited number of broken pairs. The generalized seniority concept extends this idea to multi-orbit configurations and has remained useful for understanding collective truncations with realistic interactions [6, 7].

The fermion dynamical symmetry model (FDSM) develops a related idea directly in fermion space. Collective S and D pairs are embedded in a dynamical algebra, so that collective modes arise from the symmetry properties of the underlying nucleonic system rather than being introduced as elementary bosons [8, 9, 10, 11]. The FDSM therefore offers a useful framework for asking a precise microscopic question: under what conditions can a fermionic collective Hamiltonian be represented by an effective IBM-like boson Hamiltonian?

Boson mappings address this question by constructing a correspondence between selected fermion states and operators and their images in a boson space. The mapping is not unique. Different procedures distribute the effects of the Pauli principle, finite fermion-space dimensionality, and normalization among the boson operators, the metric, and the definition of the physical subspace [12, 13, 14, 15, 16, 17, 18]. The generalized Dyson mapping is algebraically efficient and can preserve fermionic matrix elements in the physical sector, but its nonunitary nature leads in general to a non-Hermitian boson image. Seniority-based similarity transformations and Belyaev–Zelevinsky (BZ) expansions provide alternative Hermitian representations suitable for direct comparison with the conventional IBM [13, 14, 15, 16, 17, 18].

A particularly relevant study is the work of Dobeš, Navrátil, and Geyer, who investigated boson mappings of the FDSM and showed how a seniority-dictated Hermitization of the Dyson image and a BZ mapping truncated to one- and two-body terms lead to IBM-type Hamiltonians [15]. The present paper follows this physical line but focuses on the parameter systematics for even osmium isotopes and on the structural information contained in the mapped interactions.

The osmium chain is an appropriate testing ground because nuclei in this region display transitional collective behavior. IBM analyses of Pt–Os nuclei and detailed studies of ^{192}Os have long indicated a significant evolution of collective structure in this mass region [19, 20]. Modern microscopic IBM approaches based on energy-surface mapping likewise emphasize the sensitivity of collective Hamiltonians to deformation and pairing degrees of freedom [21, 23].

The aim of this work is therefore twofold. First, we formulate the Dyson, seniority, and BZ mappings of a simplified FDSM Hamiltonian in a common notation and clarify the approximations required to obtain Hermitian IBM-like operators. Second, we analyze the mapped Hamiltonian parameters for ^{186}Os , ^{188}Os , ^{190}Os , and ^{192}Os and identify the robust trends shared by different mappings. The original numerical parameter sets are retained, while the physical interpretation is formulated more cautiously: a rearrangement of effective collective interactions is distinguished from a demonstrated quantum phase transition.

2. THEORETICAL MODEL

In the approximation considered here, the collective FDSM space is generated by correlated S and D fermion pairs. The S pair carries total angular momentum $J = 0$ and represents monopole pairing, whereas the D pair carries $J = 2$ and describes quadrupole pair correlations. The restriction to these collective pairs is consistent with the general microscopic picture that low-angular-momentum pairs dominate a large part of the low-energy structure of many even-even nuclei [5, 22].

We neglect broken-pair configurations and pair scattering between normal- and abnormal-parity levels. This assumption defines the model space used for the mapping; it should not be interpreted as a statement that such configurations are absent in the physical nucleus. Within this simplified space the model admits $\text{Sp}(6) \otimes \text{SO}(2)$ and $\text{SO}(8) \otimes \text{SO}(2)$ dynamical symmetry structures, depending on the active coupling scheme [8, 9, 15].

The general proton-neutron two-body Hamiltonian in this limit contains eleven parameters. In the

original formulation used for the present application it is written as follows:

$$H_{\text{FDSM}} = \sum_{k,i} \varepsilon_{ki} n_{ki} + \sum_{a,a'} G_0^{aa'} S^\dagger(a) S(a') + G_2 D^\dagger \cdot D + \sum_{r,a,a'} B_r^{aa'} P^r(a) \cdot P^r(a') \quad (1)$$

Here ε_k and n_k are the single-particle energy and the number operator of level k (the index k labels the fermion type); a and a' label the proton and neutron subsystems; $S^\dagger(a)$ and $D^\dagger(a)$ create the collective S and D pairs of subsystem a ; $P^r(a)$ is the multipole operator of rank r ; and the dot denotes the scalar product of two tensors of equal rank.

For applications to the osmium isotopes the Hamiltonian is further reduced by retaining the dominant pairing and quadrupole terms. The resulting five-parameter form is

$$H = G_{0\pi} S_\pi^\dagger S_\pi + G_{0\nu} S_\nu^\dagger S_\nu + B_{2\pi} P_\pi^2 \cdot P_\pi^2 + B_{2\nu} P_\nu^2 \cdot P_\nu^2 + B_{2\pi\nu} P_\pi^2 \cdot P_\nu^2 \quad (2)$$

Here π and ν denote proton and neutron degrees of freedom. The first two terms represent monopole pairing in the two subsystems, while the remaining terms describe quadrupole interactions within and between the proton and neutron sectors. This reduced form preserves the competition between pairing and quadrupole collectivity that is central to the structural evolution studied below [8, 22].

2.1. Electromagnetic Quadrupole Operator

The electromagnetic quadrupole operator is taken in the one-body form

$$T(E_2) = l_\pi P_\pi^2 + l_\nu P_\nu^2 \quad (3)$$

Mapping observables is as important as mapping the Hamiltonian. Agreement in energy eigenvalues alone does not guarantee that the mapped wave functions retain the transition properties of the original fermion problem. A complete validation should therefore include $B(E2)$ values and static quadrupole moments in addition to level energies [3, 4, 5, 16]. The source calculation reports spectra and electromagnetic transition probabilities; the present paper concentrates on the mapping structure and on the parameter systematics available in the original data set. A detailed numerical calculation of the excitation spectra, $B(E2)$ values, and static quadrupole moments with the mapped Hamiltonians is reserved for future work and lies outside the scope of the present analysis of parameter evolution.

3. BOSON MAPPING OF THE FDSM OPERATORS

A boson mapping is a correspondence between a selected fermion subspace and a boson space together with a mapping of the operators acting in those spaces. The construction is subtle because the fermion space is finite and constrained by the Pauli principle, whereas the ideal boson Fock space is infinite. Consequently, the mapped boson space can contain spurious states unless a physical subspace is identified [12, 13, 14, 15, 16].

The practical objective is to reproduce fermionic matrix elements while obtaining an operator form simple enough for numerical work and comparison with the IBM. Exactness, Hermiticity, and low operator rank cannot always be achieved simultaneously. The three mappings considered below represent different compromises among these requirements.

3.1. Generalized Dyson Mapping

The FDSM Hamiltonian can be mapped onto a boson space by the generalized Dyson transformation. For the $\text{Sp}(6)$ and $\text{SO}(8)$ fermion algebras the images are expressed through s - and d -boson creation and annihilation operators. In the notation of the original model, the monopole-pair, quadrupole, dipole, and octupole operators are mapped as

$$S^\dagger \rightarrow \sqrt{\Omega} \left(s^\dagger - \frac{1}{\Omega} s^\dagger s^\dagger s - \frac{1}{\Omega} s^\dagger (d^\dagger d)^{(0)} - \frac{1}{\Omega} (d^\dagger d^\dagger)^{(0)} s - \frac{1}{\Omega} \chi ((d^\dagger d^\dagger)^{(2)} d)^{(0)} \right) \quad (4)$$

$$S \rightarrow \sqrt{\Omega} s \quad (5)$$

$$P^2 \rightarrow (d^\dagger s + s^\dagger d)^{(2)} + \chi (d^\dagger d)^{(2)} \quad (6)$$

$$P^1 \rightarrow \sqrt{2} (d^\dagger d)^{(1)}, \quad P^3 \rightarrow \sqrt{2} (d^\dagger d)^{(3)} \quad (\text{SO}(8) \text{ case}) \quad (7)$$

$$P^4 \rightarrow \frac{1}{\sqrt{2}} \sqrt{15} (d^\dagger d)^{(4)} \quad (\text{Sp}(6) \text{ case}) \quad (8)$$

In these expressions Ω denotes the fermion pair degeneracy and χ is the algebra-dependent quadrupole coefficient. The notation $(AB)^{(\lambda)}$ denotes the tensor product of the operators A and B coupled to total angular momentum λ ; in particular, $(d^\dagger d)^{(0)}$ and $(d^\dagger d^\dagger)^{(0)}$ are the scalar couplings, $(d^\dagger d)^{(2)}$ is the quadrupole coupling, and $((d^\dagger d^\dagger)^{(2)} d)^{(0)}$ couples three d -boson operators to a scalar[cite: 6]. The normalization and phase conventions of these couplings are those of Ref.[15] In the same notation $n_s = s^\dagger s$ is the s -boson number operator. The equations have been retained from the original manuscript because their normalization and phase conventions are part of the model definition.

To diagonalize the Dyson-mapped Hamiltonian, the physical boson basis must be selected consistently. The mapping is constructed so that the physical matrix elements agree with those obtained in the fermion space. However, because the Dyson transformation is nonunitary, the image of a Hermitian fermion Hamiltonian is generally non-Hermitian with respect to the standard boson scalar product [12, 13, 14, 15].

This feature distinguishes the Dyson image from the conventional Hermitian IBM Hamiltonian. It does not imply that the mapping is physically incorrect: within the physical subspace the fermionic information can be preserved. Nevertheless, for direct comparison with an IBM parametrization it is desirable to construct a Hermitian equivalent or approximation. This motivates the seniority and BZ procedures discussed next.

3.2. Seniority Mapping and Hermitization

In a seniority-based mapping, fermion states with well-defined seniority ν are related directly to boson states with a fixed number of d bosons. The simplest correspondences are

$$|N, \nu = 0\rangle \leftrightarrow |n_s = N\rangle \quad (9)$$

$$|N, \nu = 2\rangle \leftrightarrow |n_s = N - 1, n_d = 1\rangle \quad (10)$$

The purpose of this construction is to remove the mixture of different d -boson numbers that can occur in a Dyson image of a state with fixed fermion seniority. The images of the S -pair creation and annihilation operators are constrained by

$$S^\dagger \rightarrow \sqrt{\Omega} \left(s^\dagger - \frac{1}{\Omega} s^\dagger s^\dagger s - \frac{2}{\Omega} s^\dagger (d^\dagger d)^{(0)} \right) \quad (11)$$

$$S \rightarrow \sqrt{\Omega} s \quad (12)$$

For the $SU(2)$ pairing subalgebra these expressions provide a Hermitian boson image of the fermion pairing Hamiltonian. Other mapped operators can then be obtained by imposing the appropriate commutation relations or by a similarity transformation from their Dyson images. In general such transformations can generate infinite series, but the lowest orders are sufficient for the IBM-like approximation considered here [13, 15].

For the quadrupole operator the seniority image is

$$P_c^2 = (s^\dagger d)^{(2)} + \left(1 - \frac{n_s}{\Omega + 1 - 2N + 2n_s}\right) (d^\dagger s)^{(2)} + \chi \left(1 - \frac{2n_s}{\Omega - 2N + 2n_s}\right) (d^\dagger d)^{(2)} \quad (13)$$

The two-body terms in Eq. (13) contain the s -boson number operator [cite: 6]. The total number of fermion pairs, and therefore the total boson number N , is fixed. To reduce the quadrupole image to an effective one-body form, two approximations are considered. In seniority mapping A, the s -boson number operator is replaced by its value for the $\nu = 2$ state. In seniority mapping B, it is replaced by an expression involving the average seniority $\langle \nu \rangle$ of the principal FDSM states.

The average seniority $\langle \nu \rangle$ of the principal FDSM states is defined through the expectation value of the pair operator $S^\dagger S$:

$$\langle S^\dagger S \rangle = \frac{1}{4} (2N - \langle \nu \rangle) (2\Omega - 2N - \langle \nu \rangle + 2) \quad (14)$$

With these two prescriptions, the Hermitian quadrupole images become

$$P_{C,A}^2 = \sqrt{1 - \frac{N-1}{\Omega-1}} (d^\dagger s + s^\dagger d)^{(2)} + \chi \left(1 - \frac{2N-2}{\Omega-2}\right) (d^\dagger d)^{(2)} \quad (15)$$

$$P_{C,B}^2 = \sqrt{1 - \frac{N - \frac{1}{2}\langle \nu \rangle - 1}{\Omega - 1 - \langle \nu \rangle}} (d^\dagger s + s^\dagger d)^{(2)} + \chi \left(1 - \frac{2N - \langle \nu \rangle - 2}{\Omega - \langle \nu \rangle - 2}\right) (d^\dagger d)^{(2)} \quad (16)$$

The structure of Eq. (15) is closely related to the Otsuka–Arima–Iachello mapping, while Eq. (16) is closer in spirit to the extension in which seniority information is incorporated more explicitly [3, 4, 5, 6, 24]. These similarities support the interpretation of the seniority procedure as a microscopic bridge between the FDSM collective pair space and the standard s – d boson representation.

The seniority mapping is nevertheless an approximation once the operator dependence on boson number is replaced by a state-specific or averaged value. Its reliability must ultimately be judged by observables rather than by formal Hermiticity alone.

3.3. Belyaev–Zelevinsky Mapping

In the Belyaev–Zelevinsky method the boson images of the multipole operators have the same form as in the Dyson mapping, whereas the pair operators are constructed so as to satisfy the required commutation algebra while preserving Hermiticity [cite: 6]. The method originated as a microscopic boson expansion for anharmonic collective motion [18, 25].

In general, the image of a fermion pair operator is an infinite series in boson operator. For the present purpose we seek an IBM-like Hamiltonian containing only one- and two-body boson terms, so the BZ expansion is truncated consistently at that order. For the $SO(8)$ pairing operator the retained form is

$$S^\dagger \rightarrow s^\dagger \sqrt{\Omega - 2N} + \frac{1}{2}(s^\dagger s^\dagger - (d^\dagger d^\dagger)^{(0)})_s \frac{\sqrt{\Omega + 4} - \sqrt{\Omega - 2N}}{N + 2} \quad (17)$$

In the $SO(6)$ limit this expression reproduces the relevant low-lying matrix elements specified by the FDSM mapping. For $Sp(6)$ symmetry the corresponding expression is

$$S^\dagger \rightarrow s^\dagger \sqrt{\Omega - 3N} - \left[(d^\dagger d^\dagger)^{(0)}_s - s^\dagger n_d - 2s^\dagger s^\dagger s + \frac{\sqrt{7}}{2} (d^\dagger (d^\dagger d)^{(2)})^{(0)} \right] \frac{\sqrt{\Omega + \frac{3}{2}} - \sqrt{\Omega - 3N}}{3N + \frac{3}{2}} \quad (18)$$

Combining these expressions with their Hermitian conjugates and retaining only one- and two-body contributions yields a Hermitian boson image of the fermion pairing interaction. Thus both the seniority and BZ procedures produce practical IBM-type Hamiltonians, although the coefficients generated by the two mappings need not be identical.

Comparative studies of boson mappings have shown that OAI, BZ-Marshalek, and related expansion methods can reproduce similar low-energy results when the collective subspace is well developed, but they can differ as Pauli corrections and higher orders become more important [16]. This is precisely why comparing several mappings is useful: trends that survive the change of mapping are more likely to reflect the underlying collective structure rather than a specific parametrization.

4. EFFECTIVE BOSON HAMILTONIANS AND PARAMETER COMPARISON

After mapping, the FDSM Hamiltonian is expressed in terms of s and d bosons and can be organized into a one-body d -boson energy and two-boson interactions coupled to different angular momenta. The detailed coefficients depend on the mapping, the pair degeneracy, the boson number, and the normalization of the fermion operators. Therefore, absolute parameter values from different representations should not be compared term by term unless the corresponding operators have first been brought to a common convention.

In the original calculation the parameters were converted to a common system so that the four coefficients a_1 – a_4 of the Belyaev–Zelevinsky and seniority-A Hamiltonians correspond to analogous terms of the full $SU(6)$ boson Hamiltonian. The numerical values are retained below exactly as in the source tables.

For both the Belyaev–Zelevinsky and the seniority-A mappings the effective one- and two-body boson Hamiltonian is written in the common form

$$H_B = a_1 \hat{O}_1 + a_2 \hat{O}_2 + a_3 \hat{O}_3 + a_4 \hat{O}_4 \quad (18)$$

where a_i ($i = 1$ – 4) are the coefficients listed in Tables 2 and 3 and $\hat{O}_i$ are the corresponding boson operators.

Table 1. Parameters of the $SU(6)$ boson Hamiltonian for osmium isotopes (MeV).

A	ε	C_0	C_2	C_4	ϑ_0	ϑ_2
186	−0.25	0.20	−0.10	0.04	−0.31	0.04
188	−0.89	0	−0.03	0.11	−0.37	0.03
190	−0.23	−0.08	−0.07	0.09	−0.27	0.03
192	−1.98	0.78	0.16	0.41	0.60	0.20

Table 2. Parameters of the Belyaev–Zelevinsky Hamiltonian for osmium isotopes (MeV). The coefficients a_1 – a_4 multiply the boson operators $\hat{O}_1$ – $\hat{O}_4$ defined in Eq. (19).

A	a_1	a_2	a_3	a_4
186	2.01	0.70	0.25	0.02
188	2.10	0.74	0.27	0.04
190	2.15	0.80	0.32	0.05
192	1.30	0.39	0.10	0.18

Table 3. Parameters of the seniority-A Hamiltonian for osmium isotopes (MeV). The coefficients a_1 – a_4 multiply the boson operators $\hat{O}_1$ – $\hat{O}_4$ defined in Eq. (19).

A	a_1	a_2	a_3	a_4
186	2.27	1.02	0.52	0.12
188	2.35	1.05	0.58	0.14
190	2.54	1.12	0.59	0.18
192	0.65	1.14	0.62	0.21

5. RESULTS

Belyaev–Zelevinsky parameter evolution. For ^{186}Os – ^{190}Os , the first three BZ parameters change gradually: a_1 increases from 2.01 to 2.15 MeV, a_2 from 0.70 to 0.80 MeV, and a_3 from 0.25 to 0.32 MeV. The fourth parameter also increases, but remains small, from 0.02 to 0.05 MeV. This behavior is consistent with a progressive modification of the effective collective interaction as neutrons are added.

At ^{192}Os the pattern changes. The first three parameters decrease to 1.30, 0.39, and 0.10 MeV, respectively, whereas a_4 increases to 0.18 MeV. The simultaneous rearrangement of several coefficients is more informative than a fluctuation in a single parameter because it indicates a change in the balance among different components of the effective Hamiltonian.

Seniority-A Parameter Evolution. In the seniority-A representation, a_1 rises from 2.27 MeV in ^{186}Os to 2.54 MeV in ^{190}Os and then drops sharply to 0.65 MeV in ^{192}Os . By contrast, a_2 and a_3 continue a smoother increase, and a_4 changes from 0.12 to 0.21 MeV across the chain. Thus the first coefficient is especially sensitive to the transition from $A = 190$ to $A = 192$ in this mapping.

The BZ and seniority-A procedures do not yield the same numerical coefficients, as expected from their different construction. Nevertheless, both identify ^{192}Os as the isotope at which the preceding smooth trend is interrupted. This mapping-independent feature is the central numerical observation of the present analysis.

Comparison with the SU(6) Boson Parametrization. The SU(6) parameter set also changes strongly at $A = 192$. The one-boson parameter ε reaches -1.98 MeV, C_0 changes to 0.78 MeV, C_4 rises to 0.41 MeV, and v_2 changes sign and becomes 0.60 MeV. Because the SU(6), BZ, and seniority-A Hamiltonians are not identical parametrizations, a direct equality of coefficients is neither expected nor required. The relevant observation is that the isotope at which the trends reorganize is common to the three descriptions.

The numerical evidence therefore supports a structural rearrangement of the effective collective interaction near ^{192}Os . The source manuscript associated this behavior with a change of nuclear shape. In the present revision we retain the observation but avoid treating the parameter discontinuity by itself as proof of a specific prolate-to-oblate quantum phase transition.

6. DISCUSSION

The Pt–Os region has long been recognized as a transitional area in algebraic collective models. Bijker, Dieperink, Scholten, and Spanhoff described the Pt and Os isotopes within the IBM and demonstrated systematic changes of the collective Hamiltonian across the region [19]. A detailed experimental study of ^{196}Os by Casten and collaborators interpreted its level structure as the transition between the $O(6)$ limit and a symmetric rotor [20]. These independent studies provide a physical context for the parameter rearrangement found here.

The FDSM offers a complementary interpretation because the collective pairs remain explicitly fermionic before mapping. Consequently, the Pauli principle, pair degeneracy, and valence-particle number enter the construction before the effective boson Hamiltonian is obtained. The $Sp(6)$ FDSM has itself been shown to exhibit changes of intrinsic geometry as a function of valence-particle number, including axial-to-triaxial evolution caused by finite-space and Pauli effects [9]. This makes the structural sensitivity of mapped parameters physically plausible.

Nevertheless, several distinct concepts must be separated. Gamma softness, stable triaxiality, prolate-oblate evolution, and a quantum phase transition are not synonymous. A discontinuity or rapid variation in fitted or mapped Hamiltonian parameters can signal a change of effective dynamics, but classification of the nuclear shape requires observables that are directly sensitive to the wave functions.

For the present isotope chain, the next essential test is a uniform calculation of the level schemes and electromagnetic properties with the same mapped Hamiltonians. Useful indicators include $R_{4/2} = E(4_1^+)/E(2_1^+)$, the excitation energies of 0_2^+ and 2_2^+ states, odd-even staggering in the gamma band, $B(E2)$ branching ratios, and static quadrupole moments. The original study states that spectra and electromagnetic transition probabilities were obtained, but the available source tables used in this revision contain only the Hamiltonian parameters. Therefore, no new numerical $B(E2)$ values are introduced here. The detailed numerical calculation of these observables is reserved for future work; the present study is deliberately limited to the analysis of the evolution of the mapped Hamiltonian parameters.

A second issue is the truncation of the BZ expansion. Higher-order boson terms can encode Pauli corrections and the finite dimension of the underlying fermion space [13, 15, 16, 25]. If these terms become more important in a transitional nucleus, a one- and two-body truncation may require additional renormalization. The agreement of the location of the parameter rearrangement in two different Hermitian mappings is encouraging, but a quantitative uncertainty analysis would strengthen the conclusion.

A third issue concerns the microscopic interpretation of effective IBM parameters. Modern approaches map self-consistent mean-field or density-functional energy surfaces onto an IBM Hamiltonian [21, 23]. These energy-surface mappings differ formally from the operator mappings used here, but both approaches seek to connect bosonic collective dynamics with nucleonic structure. The density-functional framework has also been

extended to include pairing vibrations, emphasizing that shape and pairing collective coordinates can be coupled [23]. Such developments suggest a useful future comparison with the FDSM, where pairing is present explicitly in the starting Hamiltonian.

The principal result of this work is therefore deliberately stated at the level supported by the available calculations: the effective boson parameters obtained from different mappings evolve smoothly for ^{186}Os – ^{190}Os and undergo a pronounced reorganization at ^{192}Os . This behavior is consistent with a change of collective structure in the same mass region where independent IBM and spectroscopic studies find transitional behavior [19, 20]. Determining the precise geometric character of that change

requires the additional observables listed above.

Recent studies provide additional context for the structural evolution in the $A \approx 190$ region. Spectroscopy and lifetime measurements in ^{188}Os , interpreted with a density-functional-theory-based interacting boson-fermion model, were used to investigate the predicted prolate-to-oblate transition around $A \approx 190$ [26]. A 2024 study of neutron-rich $Z = 76$ isotopes likewise describes the osmium chain as shape transitional and finds competing prolate and triaxial structures [27]. More broadly, the mapped interacting boson model has recently been reviewed as a microscopic framework for shape transitions and coexistence in medium-heavy and heavy nuclei [28]. Beyond-mean-field calculations published in 2025 also point to enhanced prolate-oblate coexistence near $N = 116$ in rare-earth chains including Os, with quadrupole and hexadecapole collective degrees of freedom becoming strongly coupled [29]. These results strengthen the motivation for testing the present FDSM-to-boson mapping against explicit spectroscopic observables rather than inferring a unique equilibrium shape from Hamiltonian parameters alone.

7. CONCLUSIONS

We have reformulated the boson mapping of a simplified fermion dynamical symmetry model and analyzed its application to the even osmium isotopes ^{186}Os , ^{188}Os , ^{190}Os , and ^{192}Os . Three mappings were considered: the generalized Dyson mapping, a seniority-based Hermitization, and the Belyaev–Zelevinsky expansion.

The Dyson mapping provides an algebraically compact representation and preserves the relevant fermionic matrix elements in the physical boson subspace, but the mapped Hamiltonian is generally non-Hermitian in the conventional boson metric. The seniority and BZ procedures provide Hermitian IBM-like representations when the boson expansion is reduced to one- and two-body terms.

The mapped parameter sets display a common trend. Their evolution is comparatively smooth from ^{186}Os to ^{190}Os , whereas several coefficients change markedly at ^{192}Os . Because this feature appears in more than one mapping and is also reflected in the $\text{SU}(6)$ boson parametrization, it is interpreted as evidence for a rearrangement of the effective collective interaction near $A = 192$.

The present analysis does not identify the parameter rearrangement alone with a confirmed quantum phase transition. A stronger conclusion requires a systematic calculation of excitation spectra, $B(E2)$ values, quadrupole moments, and, where possible, collective energy surfaces. Such an extension would provide a direct quantitative test of how the microscopic fermion-pair structure is encoded in the effective boson description.

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ELECTROMAGNETIC PROPAGATION AND OPERATING-SYSTEM EFFECTS ON IEEE 802.11AX WI-FI PERFORMANCE

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Abstract. This paper presents a comparative analysis of the performance of IEEE 802.11ax (Wi-Fi 6) wireless Wi-Fi networks in GNU/Linux and Windows 11 environments. The focus is on throughput, data transfer latency, CPU load, and RAM usage. The study was carried out using simulation modeling using identical hardware and radio environment conditions for both operating systems. The obtained results show that the architectural features of network subsystems have a significant impact on connection quality metrics, in particular: GNU/Linux demonstrates higher throughput and lower latency, while Windows 11 has a higher CPU load and RAM consumption. The work has practical significance for choosing an operating system when building highly efficient Wi-Fi networks.

Keywords: Wi-Fi 6, GNU/Linux, Windows 11, throughput, latency, CPU usage, RAM usage, network subsystems, simulation.

1. INTRODUCTION

Wireless data transmission technologies are a key element of modern telecommunications systems. WLAN occupies a special place and is used in home, commercial, and educational networks [1, 2]. The development of the IEEE 802.11 standard has led to a significant increase in data transfer rates and improved connection stability [3].

An analysis of current scientific publications shows that studying the characteristics of IEEE 802.11ax (Wi-Fi 6) wireless networks is an important area of research in telecommunications. Current research focuses on protocol mechanisms, radio resource efficiency, and quality of service.

At the physical layer, an IEEE 802.11ax link is an electromagnetic-wave system. Its measured throughput and latency depend on received power and signal-to-noise ratio, which are governed by geometric spreading, absorption, reflection, diffraction, scattering, and coherent addition of multipath components. The free-space wavelengths are approximately 0.125 m at 2.4 GHz and 0.060 m at 5 GHz. Consequently, the 5 GHz band has 6.38 dB greater free-space path loss than 2.4 GHz at the same distance and antenna gains, while its shorter wavelength also makes propagation more sensitive to surface roughness, apertures, and obstruction geometry [3, 4].

Cristobo L., Zabala I., Ibarrola E., and Ferro A. present the results of a study on the implementation of Wi-Fi 6 in a university campus infrastructure. They demonstrated that the use of the IEEE 802.11ax standard improves QoS and QoE performance in networks with high user density, especially when analyzing network parameters using machine learning methods. However, questions about the impact of the programming environment and operating system architecture on wireless connection characteristics remain unanswered. This may be due to the fact that the study mainly focused on network infrastructure and radio resource management methods [4].

Mozaffari-khor E., Theoleyre F., and Menth M. present an overview of key technologies in the IEEE 802.11ax standard, including OFDMA, MU-MIMO, and Target Wake Time. These technologies have been shown to increase throughput, reduce data transmission latency, and improve the

energy efficiency of wireless devices. However, the impact of the implementation of operating system network protocol functions on wireless channel performance remains unclear. This is because research to date has focused primarily on the protocol and physical layers of network architecture [5].

Boris Bellalta's article presents the results of research into performance-enhancing mechanisms for IEEE 802.11ax networks, including the use of OFDMA technology and interference management techniques. These mechanisms were shown to improve spectral efficiency and reduce interference between users. However, the impact of programming environments and network operating systems on the actual performance of wireless networks remains unclear. This is because the research has focused on optimizing the standard's protocol mechanisms [6].

Evgeny Khorov presents the results of an analysis of the multiple access mechanisms of the IEEE 802.11ax standard. The analysis showed that the use of OFDMA technology significantly improves network performance at high device densities. However, questions about the impact of operating system architecture and network driver implementation on wireless connection performance remain unanswered. This is due to the fact that the study primarily focused on protocol-level analysis [7].

Therefore, research has primarily focused on the IEEE 802.11ax protocol mechanisms and radio resource allocation optimization. However, the impact of operating system architectures, such as Linux and Windows 11, on wireless network performance remains understudied. Modern operating systems implement various network stacks and drivers that affect WLAN performance [8, 9, 10].

All this suggests that a comparative study would be useful for analyzing the performance characteristics of IEEE 802.11ax wireless networks in various software environments, especially in GNU/Linux and Windows 11 operating systems. This study would help identify the specific performance characteristics of wireless networks in various environments and determine the factors affecting the performance of wireless LANs in modern computer systems.

The objective of this study is to determine how fundamental indoor electromagnetic-wave mechanisms and operating-system network-stack implementations jointly shape IEEE 802.11ax performance in GNU/Linux and Windows 11. The analysis distinguishes physical-channel effects (frequency, distance, material boundaries, and multipath propagation) from software-platform effects on throughput, RTT, CPU load, and RAM usage.

Research objectives:

1. To analyze current scientific publications devoted to the study of the characteristics of wireless networks of the Wi-Fi 6 standard based on the IEEE 802.11ax standard, and to identify the main directions and limitations of existing research.
2. To examine the architectural features of network stacks of GNU/Linux and Windows 11 operating systems and determine their impact on the operation of wireless network interfaces.
3. To develop a methodology for experimental testing of wireless connection properties in various software environments.
4. To conduct a comparative experimental study of the parameters of a Wi-Fi wireless network in the GNU/Linux and Windows 11 operating systems.
5. To evaluate and compare the main performance indicators of a wireless connection (throughput, data transmission latency, connection stability) for the studied software environments.
6. Formulate conclusions and recommendations on the use of various operating systems to improve the efficiency of wireless networks of the IEEE 802.11ax standard.

2. HARDWARE AND SOFTWARE CONFIGURATION FOR THE EXPERIMENTAL SIMULATION

A simulated hardware and software configuration compliant with the current Wi-Fi 6 standard is used to build the model.

The following setup is considered as the baseline configuration:

1. Laptop with Ubuntu 24.04 LTS [16];
2. Laptop with Windows 11 Pro [15];
3. Intel AX210 Wi-Fi adapter [13, 14];
4. Wi-Fi 6 access point [1];
5. Second computer for the server component.

Accepted radio environment parameters:

1. Infrastructure connection mode (STA $\leftrightarrow$ AP);
2. Channel width 80 MHz;
3. Frequency range 5 GHz;
4. Distance to the access point up to 5 meters;
5. WPA3-Personal encryption mode;
6. Minimal external interference.

Selecting the same adapter and access point eliminates the influence of hardware differences and focuses on software factors.

The simulation assumes that:

- the signal level is stable;
- there is no channel change;
- there is no BSS congestion;
- there are no background downloads unrelated to the experiment.

This configuration ensures reproducible results and accurate comparative analysis.

3. RESEARCH METHODS

The operating systems were compared using matched scenarios: run i under GNU/Linux corresponds to the same modeled radio conditions as run i under Windows 11. This pairing controls the scenario-level variation and isolates the software-platform difference as far as the available design permits [11].

Simulation method: ten stochastic runs were generated for each operating system using bounded perturbations of throughput, RTT, CPU load, and RAM usage. The original description 'discrete-event simulation' was imprecise because the reported model generates one metric vector per run and does not define an event calendar. Statistical post-processing of the tabulated paired runs in this revision was performed in Python 3.12 with NumPy and SciPy.

Testbed and statistical analysis: all comparisons used the same access point, client computer, Wi-Fi adapter, channel settings, and transmitter-receiver geometry.

Results are reported as mean $\pm$ sample standard deviation. Paired, two-sided t-tests assessed $H_0: \mu_d = 0$ at $\alpha = 0.05$; Holm's procedure controlled the family-wise error rate across four endpoints, and Cohen's d_z quantified paired effect size [5, 6].

4. PHYSICAL MODEL OF INDOOR RADIO-WAVE PROPAGATION

For a linear, isotropic medium, the macroscopic electromagnetic field obeys Maxwell's equations. With $\mathbf{D} = \epsilon \mathbf{E}$, $\mathbf{B} = \mu \mathbf{H}$, and conduction current $\mathbf{J} = \sigma \mathbf{E}$, they lead to the lossy-medium wave equation [3, 4]:

$$\nabla \times \mathbf{E} = -\partial \mathbf{B} / \partial t, \quad \nabla \times \mathbf{H} = \sigma \mathbf{E} + \partial \mathbf{D} / \partial t, \quad \nabla \cdot \mathbf{D} = \rho, \quad \nabla \cdot \mathbf{B} = 0, \quad (1)$$

$$\nabla^2 \mathbf{E} - \mu \sigma (\partial \mathbf{E} / \partial t) - \mu \epsilon (\partial^2 \mathbf{E} / \partial t^2) = 0. \quad (2)$$

The frequency f fixes the free-space wavelength $\lambda = c/f$. Thus $\lambda \approx 0.125$ m at 2.4 GHz and $\lambda \approx 0.060$ m at 5 GHz. For equal distance and antenna gains, the free-space received power decreases with frequency because $\text{FSPL} = 20 \log_{10}(4\pi d/\lambda)$; the 5-to-2.4 GHz difference is $20 \log_{10}(5/2.4) = 6.38$ dB:

$$\lambda = c/f, \quad \text{FSPL}(d, f) = 20 \log_{10}(4\pi d f / c). \quad (3)$$

Material loss is represented by complex relative permittivity. Its real part describes electric-field energy storage and phase velocity, whereas conductivity contributes to the imaginary (loss) component:

$$\epsilon_r^* = \epsilon_r' - j\sigma/(\omega\epsilon_0), \quad \tan \delta = \sigma/(\omega\epsilon_0\epsilon_r'). \quad (4)$$

At an air-material boundary, the impedance discontinuity produces a reflected wave and a transmitted wave. For normal incidence between non-magnetic media, a compact field-amplitude relation is:

$$\Gamma = \frac{\sqrt{\epsilon_{r1}^*} - \sqrt{\epsilon_{r2}^*}}{\sqrt{\epsilon_{r1}^*} + \sqrt{\epsilon_{r2}^*}}. \quad (5)$$

At oblique incidence, the TE and TM Fresnel coefficients also depend on polarization and incidence angle. Multiple reflections from walls, floor, ceiling, furniture, and conductive objects arrive with different delays and phases; their vector sum can strengthen or weaken the received field.

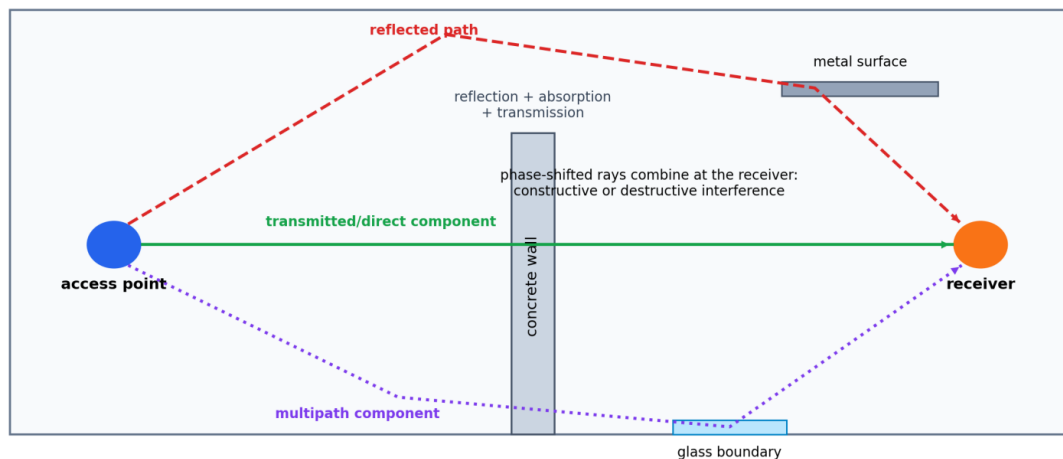


Figure 1 – Physical mechanisms of indoor radio-wave propagation

Concrete is a heterogeneous, lossy dielectric. Its moisture, pores, and aggregate interfaces cause absorption, internal reflection, and scattering. Glass has a strong permittivity contrast with air and therefore reflects part of the incident field; finite thickness creates repeated internal reflections and frequency-selective transmission. Metal has very high conductivity, so induced surface currents oppose field penetration: most incident energy is reflected and the transmitted field decays over a small

skin depth. Because conductivity of concrete and glass increases with frequency in the ITU-R model, and because free-space loss is already higher at 5 GHz, penetration is generally poorer at 5 GHz than at 2.4 GHz for the same geometry [4].

ITU-R P.2040-3 models $\epsilon'_r = af^b$ and $\sigma = cf^d$, with f in GHz. The values above use the recommendation's material-class coefficients; actual properties depend on composition, moisture, thickness, coatings, and reinforcement [?].

Large-scale indoor attenuation is summarized by the log-distance path-loss model:

$$PL(d) = PL(d_0) + 10n \log_{10}(d/d_0) + X_\sigma + \sum L_i. \quad (6)$$

Table 1. Representative electrical properties of indoor obstacles calculated from ITU-R P.2040-3 [4]

Material	ϵ'_r	σ at 2.4 GHz (S/m)	σ at 5 GHz (S/m)	Dominant physical effect
Concrete	5.24	0.0916	0.1627	Absorption, reflection, heterogeneous scattering
Glass	6.31	0.0116	0.0311	Boundary reflection and slab interference
Metal	≈ 1 (model convention)	1.0×10^7	1.0×10^7	Strong reflection; shallow skin depth

Here $PL(d)$ is the reduction in received power, expressed in decibels, at transmitter-receiver distance d ; $PL(d_0)$ is the calibrated loss at reference distance d_0 ; n is the propagation exponent and therefore represents how rapidly mean loss grows in the particular environment; X_σ is a zero-mean Gaussian shadowing term in dB that represents spatial fluctuations caused by reflections, interference, medium heterogeneity, and multipath propagation; and $\sum L_i$ collects penetration losses of specific obstacles. In free space $n \approx 2$, whereas clutter, obstruction, and lossy boundaries produce larger effective n . The relation is a statistical channel model, not a replacement for Maxwell's equations; its parameters summarize the net effect of the underlying electrodynamics.

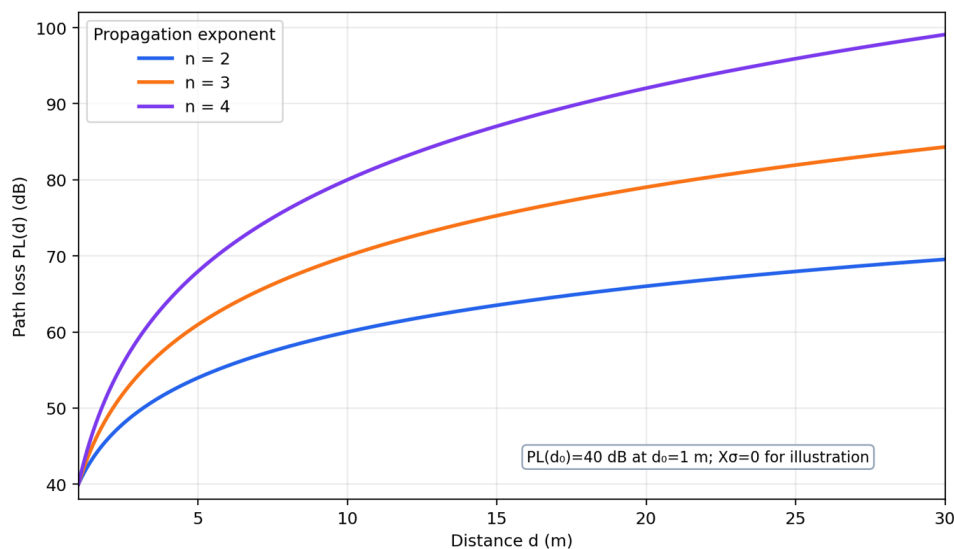


Figure 2 – Dependence of log-distance path loss on distance for different propagation exponents

Formally, the measured system is represented by the parameter vector:

$$S = \{T, L, C, M\}, \quad (7)$$

where T is the network throughput, L is the data transfer delay, C is the processor load, and M is the RAM load.

System performance was assessed using a series of paired stochastic runs. Each run $i \in \{1, 2, \dots, 10\}$ generates the observation vector:

$$S_i = \{T_i, L_i, C_i, M_i\}. \quad (8)$$

The sample mean is calculated using:

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i, \quad (9)$$

where $n = 10$.

Sampling variability is estimated by the sample standard deviation:

$$\sigma = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2}. \quad (10)$$

Bounded stochastic variability around each baseline is represented by:

$$X_i = x_{\text{base}} + \varepsilon_i, \quad (11)$$

where ε_i is a random variable with limited amplitude, reflecting the influence of radio interference, load changes and background processes of the operating system.

Thus, the study uses a stochastic paired-scenario model with bounded parameter variability; it is not characterized as a discrete-event model in the revised manuscript.

For each endpoint, $d_i = X_{i,\text{Linux}} - X_{i,\text{Windows}}$. The paired statistic and paired standardized effect are:

$$t = \bar{d}/(s_d/\sqrt{n}), \quad \text{df} = n - 1, \quad dz = \bar{d}/s_d. \quad (12)$$

The normality assumption was evaluated on paired differences using the Shapiro-Wilk test. With $n = 10$, this diagnostic has limited power and was interpreted together with the absence of extreme paired differences.

5. SIMULATION RESULTS AND ANALYSIS OF RESULTS

The study was conducted primarily using simulation modeling methods to evaluate the properties of wireless networks under controlled environmental conditions.

To partially verify the model and improve the reliability of the results, a series of experimental measurements were carried out at the Department of Radio Electronics and Telecommunications.

Measurements were conducted at a limited number of indoor test points located at varying distances from the access point. This allowed us to account for the impact of spatial signal distribution on connection parameters.

The obtained experimental data were used for qualitative comparison with the results of simulation modeling and to confirm the identified patterns.

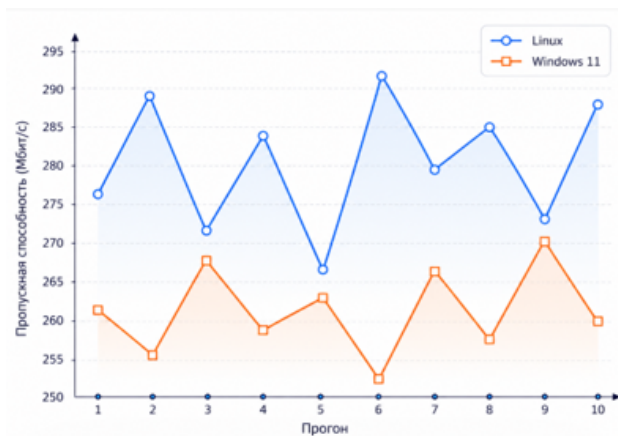
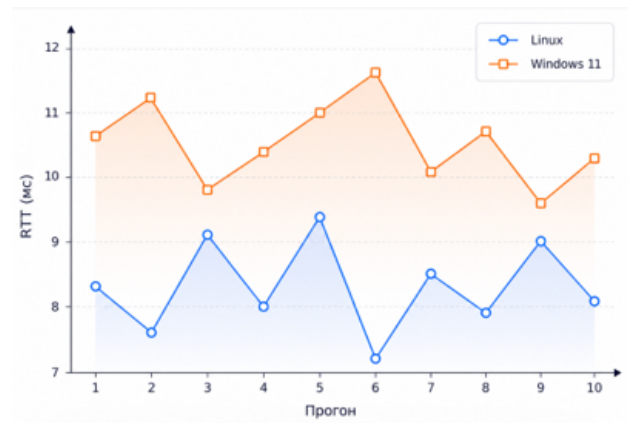
Comparative results for throughput (Mbps) and data transmission delay (RTT, ms) are presented in Table 2 and Figures 3 and 4.

Table 2. Data transfer rate and latency (RTT, ms)

Connection bandwidth (Mbps)			Data transmission delay (RTT, ms)		
Measurement No.	Linux	Windows 11	Measurement No.	Linux	Windows 11
1	276	261	1	8.3	10.7
2	289	255	2	7.6	11.2
3	271	268	3	9.1	9.8
4	284	259	4	8.0	10.4
5	267	263	5	9.4	11.0
6	292	252	6	7.2	11.5
7	279	266	7	8.5	10.1
8	285	257	8	7.9	10.8
9	273	270	9	9.0	9.6
10	288	260	10	8.1	10.3

Average throughput: Linux 280.4 ± 8.5 ; Windows 261.1 ± 5.7 .

Average data transfer delay: Linux 8.31 ± 0.70 ; Windows 10.54 ± 0.61 .

**Figure 3** – Comparative analysis of network throughput**Figure 4** – Comparative analysis of data transmission latency

Comparative results of CPU (%) and RAM (MB) usage are presented in Table 3 and illustrated in Figures 5 and 6.

Average CPU usage: Linux 13.7 ± 1.3 ; Windows 22.1 ± 1.7 .

Average amount of RAM used (MB): Linux 1121.0 ± 21.1 ; Windows 1324.5 ± 24.2 .

Formal statistical validation is reported in Table 4. All paired-difference distributions were compatible with normality at the 0.05 level (Shapiro-Wilk $p = 0.212$ – 0.897). All four OS differences remained significant after Holm correction.

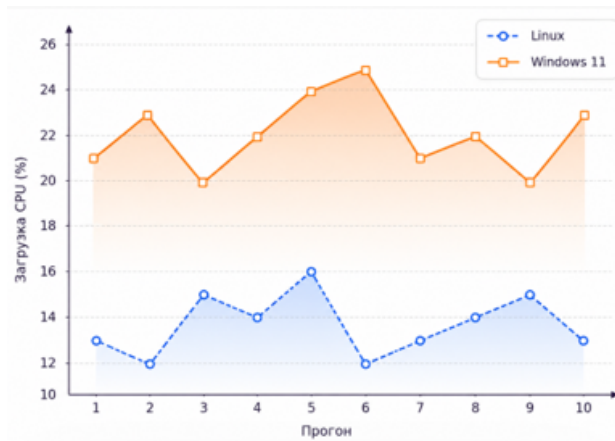
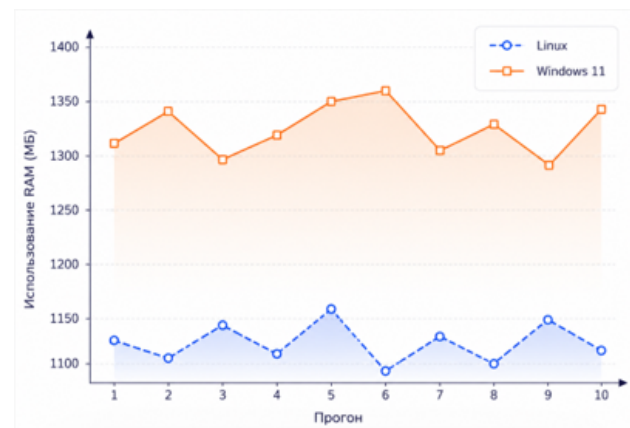
Positive differences favor GNU/Linux for throughput; negative differences indicate lower GNU/Linux values for RTT and resource use. Confidence intervals are unadjusted 95% paired intervals; p values use Holm's family-wise correction.

Table 3. CPU Usage (%) and RAM Usage (MB)

CPU Usage (%)			RAM usage (MB)		
Measurement No.	Linux	Windows 11	Measurement No.	Linux	Windows 11
1	13	21	1	1120	1310
2	12	23	2	1105	1340
3	15	20	3	1140	1295
4	14	22	4	1110	1320
5	16	24	5	1155	1350
6	12	25	6	1090	1360
7	13	21	7	1130	1305
8	14	22	8	1100	1330
9	15	20	9	1145	1290
10	13	23	10	1115	1345

Table 4. Paired two-sided t-tests for GNU/Linux minus Windows 11

Endpoint	Mean difference	95% CI	t(9)	Holm-adjusted p	dz
Throughput (Mbps)	+19.30	9.61 to 28.99	4.505	0.001479	1.42
RTT (ms)	−2.23	−3.07 to −1.39	−5.993	0.000408	1.90
CPU (%)	−8.40	−10.16 to −6.64	−10.804	0.00000562	3.42
RAM (MB)	−203.50	−231.41 to −175.59	−16.492	< 0.000001	5.22

**Figure 5** – Comparative analysis of CPU utilization**Figure 6** – Comparative analysis of RAM utilization

Analysis of results:

1. Performance: GNU/Linux provided 7.4% higher mean throughput than Windows 11. This difference may reflect more efficient packet processing and Wi-Fi management, but the design does not identify a single software mechanism [15, 16].
2. Latency: mean RTT was 2.23 ms lower under GNU/Linux; the paired comparison was significant, but the present design does not isolate scanning, roaming, driver, or scheduler contributions.

3. CPU and RAM usage: Windows 11 used 61.3% more CPU and 18.2% more RAM than GNU/Linux on average. These differences are consistent with dissimilar network-driver, filtering, and background-service architectures, although component-level causality was not tested [17].
4. Practical benefit: The results allow you to choose an operating system based on your priorities: maximum performance and stability – Linux; easy integration and built-in services – Windows 11.

The obtained data are consistent with theoretical assumptions regarding the influence of latency and buffering on data transmission delay. Resource allocation mechanisms in the IEEE 802.11ax standard directly affect latency and jitter under load [18].

Experimental studies of the IEEE 802.11ax standard have shown that using modern resource management mechanisms can reduce latency by 20–30% compared to previous generations of Wi-Fi.

Additionally, technical reviews conducted by Intel confirm lower latency and higher throughput when using Wi-Fi 6.

5.1. *Physical interpretation of the measured differences*

The paired design holds the modeled radio environment constant between operating systems; therefore, the OS contrasts in Table 4 should not be attributed to different path loss. Nevertheless, the absolute link state available to both systems is set by received field strength and multipath structure. A lower received signal-to-noise ratio increases retransmissions and modulation/coding fallback, which can magnify latency and reduce throughput before network-stack processing is considered. Thus software and propagation effects are sequential and interacting rather than interchangeable.

5.2. *Study limitations*

The sample contains only ten paired runs and a limited number of indoor validation points. Material permittivity and conductivity were used for physical interpretation rather than measured for the specific building; wall thickness, reinforcement, moisture, incidence angle, and spatial fading were not independently estimated. Consequently, the study supports the direction of the 2.4/5 GHz and obstacle effects but does not claim calibrated penetration-loss values for the tested site. Future work should report a complete reproducible testbed, measure RSSI/SNR and packet retransmissions, and fit $PL(d_0)$, n , σ , and obstacle losses separately for each band.

6. CONCLUSIONS

Conclusions were formulated based on previously defined objectives:

- An analysis of scientific publications revealed that most research on IEEE 802.11ax network development focuses on protocol mechanisms designed to improve data transmission efficiency and optimize radio resource utilization. However, the impact of the programming environment and operating system architecture on wireless network performance has not been sufficiently addressed in existing studies, highlighting the relevance of this study [19].
- An analysis of the architectures of network subsystems of the GNU/Linux and Windows 11 operating systems showed that differences in the implementation of network stacks, network queue processing mechanisms and driver subsystems can significantly affect the operating parameters of wireless interfaces [20, 21, 22].

- The revised stochastic paired-scenario methodology combines a physical channel interpretation with operating-system comparisons. The log-distance model relates distance-dependent loss to the propagation exponent and shadowing, while complex permittivity and conductivity explain reflection, absorption, and penetration through concrete, glass, and metal.
- The experiments conducted allowed us to obtain quantitative results regarding the operation of the wireless network in various software environments, as well as to identify differences in data transfer parameters between the tested operating systems.
- The GNU/Linux operating system achieved higher average throughput (280.4 Mbps) and lower data transfer latency (8.31 ms) compared to Windows 11 (10.54 ms), indicating more efficient processing of network packets and less load on the network stack.
- The obtained results demonstrate the feasibility of using GNU/Linux in efficient IEEE 802.11ax networks, while showing that network parameters are not determined by software processing alone. They also depend on electromagnetic-wave attenuation, reflection at media boundaries, multipath interference, and frequency-dependent penetration through obstacles. At equal geometry, 5 GHz begins with 6.38 dB more free-space loss than 2.4 GHz and usually experiences stronger material-related attenuation; these physical effects must be considered together with operating-system architecture when designing and interpreting indoor Wi-Fi measurements.

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