

MODELING MOISTURE TRANSPORT IN POROUS DIELECTRIC STRUCTURES FOR ADVANCED HUMIDITY SENSING IN INTELLIGENT AND ASSISTIVE SYSTEMS

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Abstract

To design high-performance humidity sensors for next-generation intelligent systems, assistive technologies, and autonomous robotic platforms, a comprehensive understanding of moisture transport processes in porous dielectric materials is essential. Moisture sensing plays a critical role in environmental monitoring, healthcare applications, smart infrastructure, and robotic systems operating in dynamic environments. In porous structures containing nanoscale and micro-scale pores, water vapor transport is governed by both molecular diffusion and Knudsen diffusion, making conventional diffusion models inadequate when pore dimensions approach the molecular mean free path. This work employs the Bosanquet approximation to capture the combined effects of molecular and Knudsen diffusion and performs a numerical investigation of moisture transport in porous dielectric structures. Parametric simulations are conducted for pore radii ranging from 50 nm to 1000 nm under standard operating conditions. The influence of pore size on Knudsen diffusion, effective diffusion coefficients, and transport resistance is systematically analyzed. Results reveal a transition diffusion regime in which both molecule–molecule and molecule–wall interactions significantly affect transport behavior. The findings demonstrate that pore geometry strongly influences moisture transport characteristics and provide valuable design insights for the development of advanced humidity sensors and sensing systems supporting assistive technologies, smart environments, robotic perception, and future autonomous monitoring applications.

1. INTRODUCTION

Humidity sensors find widespread applications in industrial process control, environmental monitoring, semiconductor manufacture, pharmaceutical processing, and in aerospace systems [1-5]. A porous dielectric humidity sensor

has moisture transport (Figure 1) through its porous sensing layer that influences its performance significantly [6-9]. Water molecules need to migrate through the network of pores to reach the active sensing sites for adsorption to reach equilibrium [10-13].

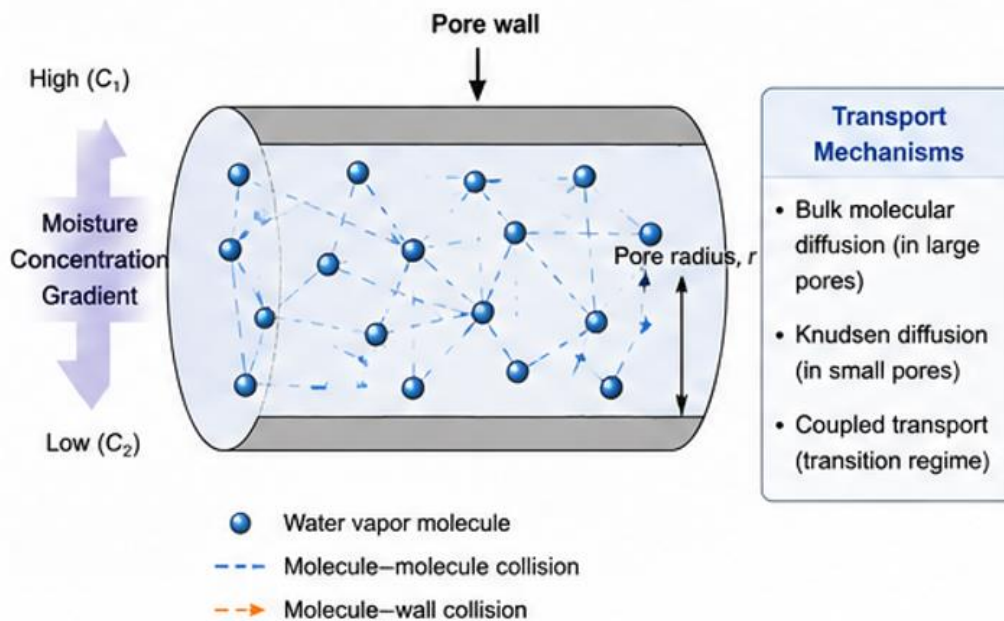


Figure 1: Moisture Transport Mechanism in a cylindrical pore under a concentration gradient

When pore sizes fall into the nanometer regime, the transport of water vapor within porous materials becomes more complicated. In this case, the classical molecular diffusion theory is no longer applicable as the movements of molecules are greatly affected by collisions with the walls of the pores [12-13]. The Bosanquet approximation is a combination of bulk molecular diffusion and Knudsen diffusion into a single effective diffusion coefficient to accurately model this behavior. In this paper, this model is numerically studied and the effects of pore size on moisture transport properties are investigated.

2. THEORY OF DIFFUSION IN POROUS STRUCTURES

The transfer of moisture in porous substances happens because of concentration gradients. There are two ways diffusion may take place, depending upon the pore size [14-20].

2.1 Molecular Diffusion

In large pores the water molecules have more collisions with each other. The process occurs by Fickian diffusion, and is determined by the bulk diffusion coefficient [21].

If the water vapor is present in air:

$$D_b = 2.42 \times 10^{-5} m^2/s$$

When the pore diameters are significantly larger than the mean free path of the molecules, the temperature is room temperature, and molecular diffusion is dominant.

2.2 Knudsen Diffusion

If the dimension of the pores is similar to the molecular mean free path, the behavior of transport is controlled by the collisions with the pores wall.

The Knudsen diffusion [22] coefficient is:

$$D_k = \frac{2r}{3} \sqrt{\frac{8RT}{\pi M}}$$

This equation is valid only when r is the pore radius, R the gas constant, T the temperature and M the molecular mass. Figure 2 shows illustration of Knudsen diffusion [22] coefficient, there it has been shown that Dk increases with pore radius.

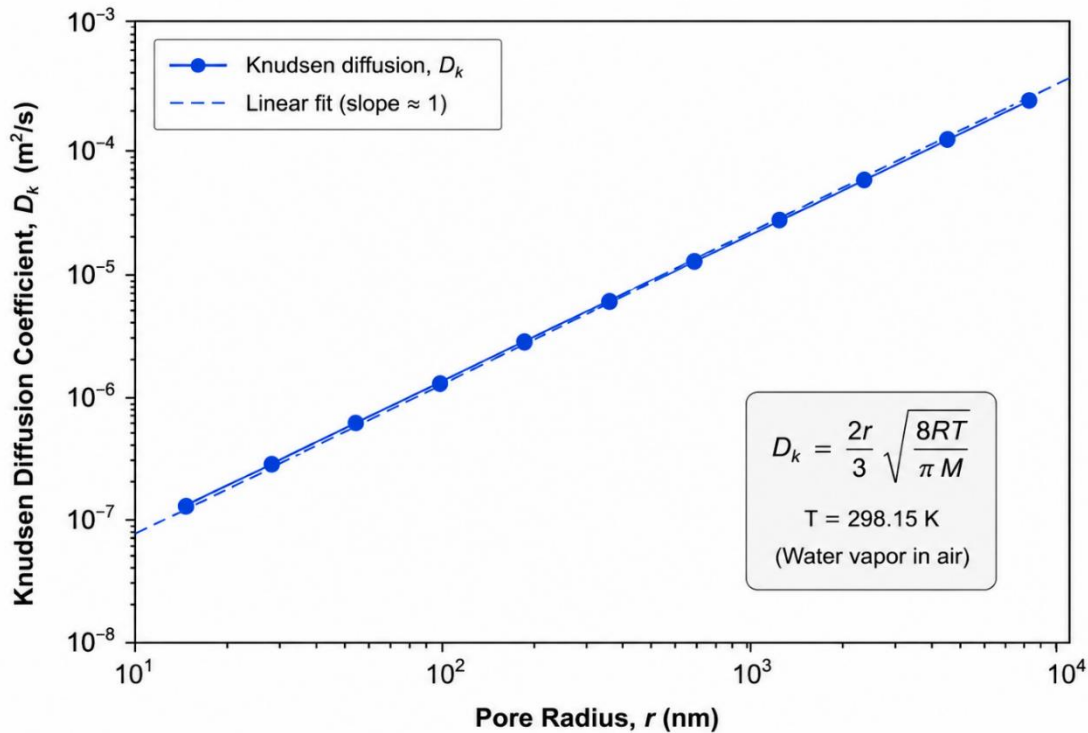


Figure 2: Knudsen Diffusion Coefficient as a function of pore radius (log-log scale), Dk increases with pore radius.

3. BOSANQUET APPROXIMATION

The Bosanquet approximation is a mixture of both transport mechanisms [21-26]:

$$\frac{1}{D_{eff}} = \frac{1}{D_b} + \frac{1}{D_k}$$

or

$$D_{eff} = \frac{D_b D_k}{D_b + D_k}$$

It is assumed that both the transport resistances operate concurrently and the slowest of them dominates the overall transport.

Figure 3 shows the variation of the diffusion coefficient (D) of a gas with pore radius (r) in a porous medium. It is specifically designed to identify smooth transition between two different physical mechanisms of

diffusion over three characteristic regimes, the Bosanquet approximation. This is the detailed explanation of the parts and the physics exhibited in figure 3.

3.1 The three Diffusion Coefficients:

Bulk Molecular Diffusion (D_b , Green Dashed Line in figure 3): Classical Gas Diffusion - molecule-to-molecule collisions dominate. It is not dependent on the physical geometry of the container, but rather only on temperature, pressure and the specific gas mixture and is thus the same for all pore sizes.

Knudsen Diffusion (D_k , Blue Dashed Line in figure 3): This is when the pore size is less than or about the same as the mean free path of the gas molecules, so that the molecules are liable to

bump into the walls of the pores far more often than each other. Mathematically, D_k is directly proportional to the pore radius, and this is represented as a straight diagonal line on this log-log plot.

Effective diffusion coefficient (D_{eff} , Red Solid Line in figure 3): This is the diffusion coefficient as determined in real conditions with the Bosanquet approximation. It harmonizes both mechanisms based on inverse addition rule:

$$\frac{1}{D_{eff}} = \frac{1}{D_k} + \frac{1}{D_b}$$

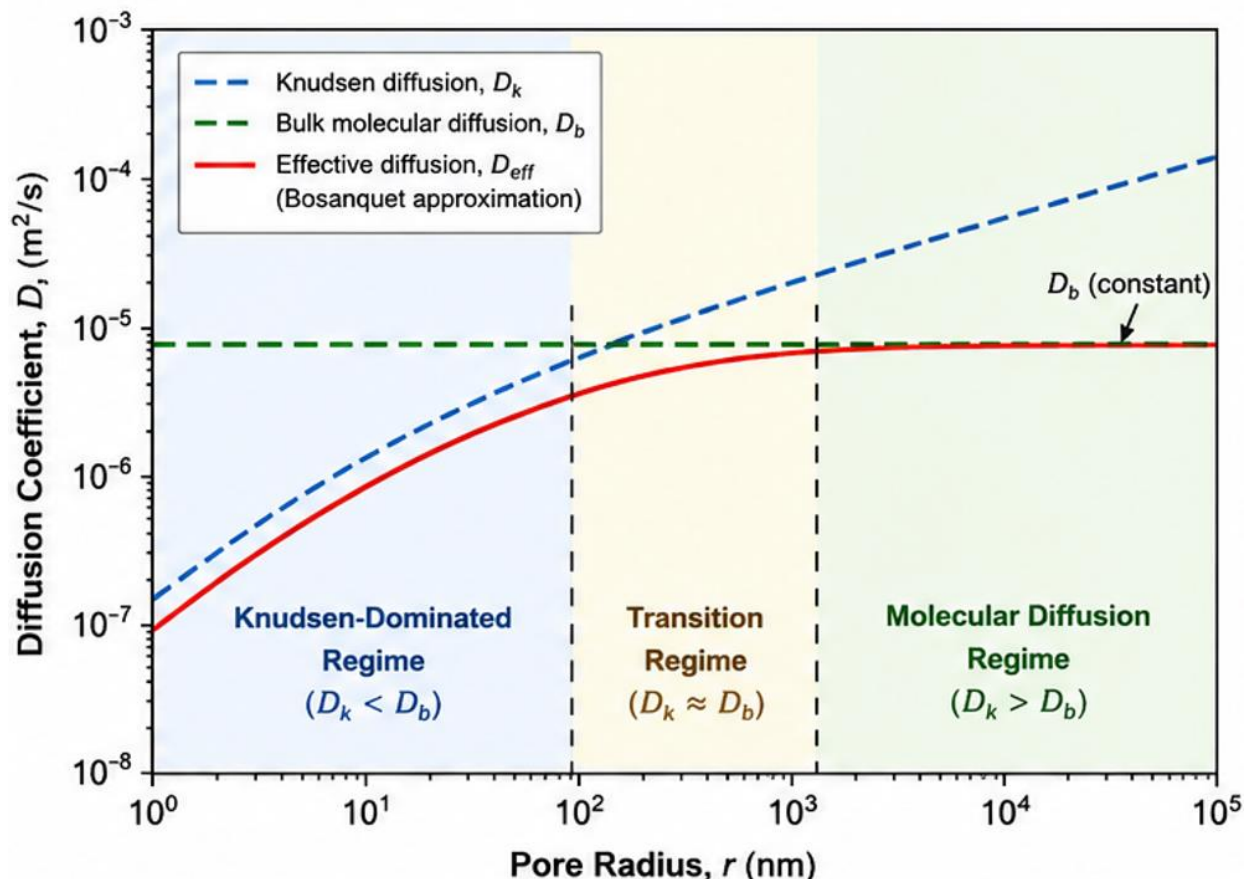


Figure 3: Comparison of D_k , D_b , and D_{eff} as a function of pore radius showing Knudsen-Dominated, Transition, and Molecular Diffusion Regimes.

3.2 The Three Transport Regimes

The graph is plotted in three different zones corresponding to a pore radius (r):

Knudsen-Dominated Regime ($r < 100$ nm): In very fine pores, molecules move in the pore itself with significant restriction in the pore walls. The

inverse sum is dominated by the Knudsen term since $D_k \ll D_b$ and $D_{eff} \approx D_k$. Notice that the solid red line here perfectly matches the blue dashed line. In the transition regime ($100 \text{ nm} \leq r \leq 1300 \text{ nm}$), the probability of the molecule colliding with another molecule is estimated to be the same as the probability of colliding with the pore wall ($D_k \approx D_b$). Both mechanisms must be taken into account. The Bosanquet approximation (red line) is a smooth function that lies below both of the individual limits, as it represents the resistance to transport when the two are combined. Molecule to molecule interactions determine the transport in the larger macropores, in the Molecular Diffusion Regime ($r > 1300 \text{ nm}$). As $D_k \gg D_b$ the effective diffusion is approximately constant at the bulk diffusion limit ($D_{eff} \approx D_b$) and stays constant along the green dashed line. Figure 3 supports visually the usefulness of the Bosanquet approximation. The approximation allows for a continuous, highly accurate pore structural approximation spanning five orders of magnitude of pore structural scaling with no need to use

separate and discontinuous mathematical descriptions for small and large pores.

4. NUMERICAL METHODOLOGY

The numerical calculations were carried out in MATLAB.

Assumptions:

- Temperature = 298.15 K
- Pressure = 1 atm

The water vapour is the diffusing species.

- Molecular weight of water = 0.018015 kg/mol
- Bulk diffusion coefficient = $2.42 \times 10^{-5} \text{ m}^2/\text{s}$

Pore radii considered are given below:

- 50 nm
- 100 nm
- 200 nm
- 500 nm
- 1000 nm

Knudsen diffusion and effective diffusion coefficients for each radius were determined.

5. RESULTS

5.1 Knudsen Diffusion Coefficient

The numerical calculations obtained the results that the Knudsen diffusion increases linearly with the pore radius (table 1).

Table 1. Knudsen Diffusion Coefficients

Radius (nm)	D_k (m ² /s)
50	1.97×10^{-5}
100	3.94×10^{-5}
200	7.88×10^{-5}
500	1.97×10^{-4}
1000	3.94×10^{-4}

These results confirm that the Knudsen diffusion coefficient is directly proportional to the pore radius. The larger the size of the pores, the less frequent will be the collisions between the walls, the more unrestricted the flow of moisture will be.

5.2 Effective Diffusion Coefficient

Using the Bosanquet approximation we obtain effective diffusion coefficients in table 2.

Table 2. Effective Diffusion Coefficients

Radius (nm)	D_{eff} (m ² /s)
50	1.08×10^{-5}
100	1.50×10^{-5}
200	1.84×10^{-5}

500	2.16×10^{-4}
1000	2.28×10^{-4}

As the pore radius increases, the effective diffusion coefficient (D_{eff}) gets closer to the bulk diffusion coefficient (D_b). It can be seen in figure 4.

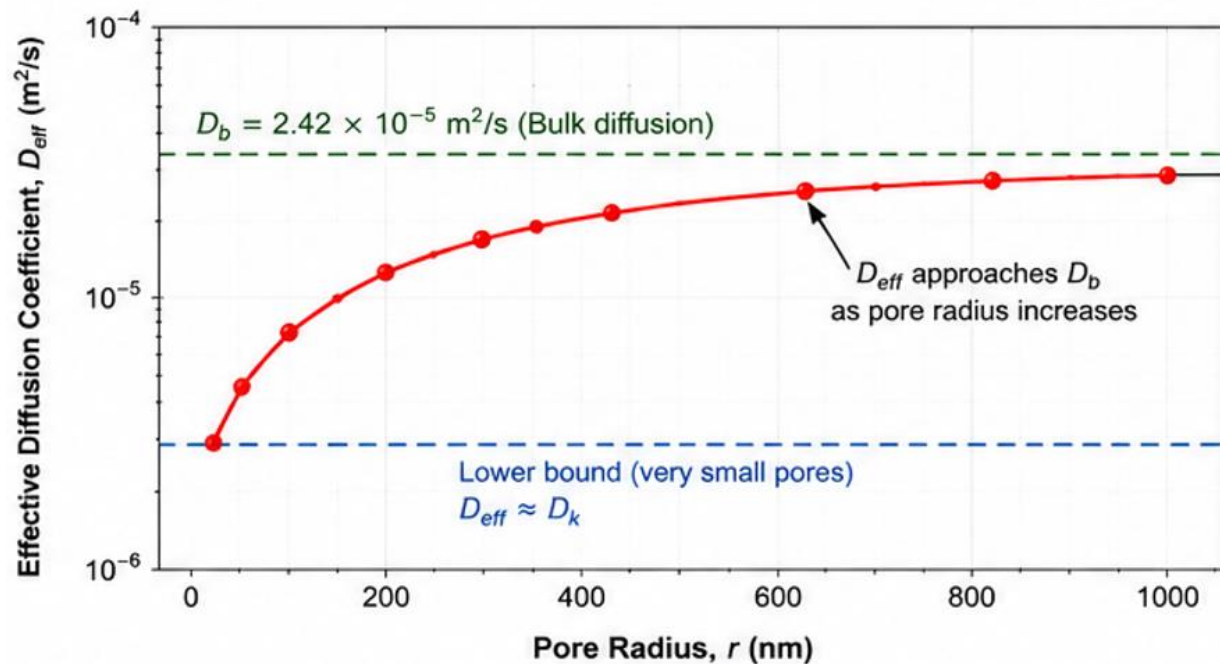


Figure 4: Effective Diffusion Coefficient calculated using Bosanquet Approximation as a function of pore radius

6. DISCUSSION

The numerical results clearly show three regimes of diffusion.

6.1 Knudsen-Dominated Regime

At the pore size of 50 nm, D_k is smaller than D_b . Molecule-wall interactions are very limiting for transport. This is a considerable decrease in the effective diffusion coefficient.

6.2 Transition Regime

At pore radii between 100 and 500 nm, D_k and D_b are now similar. Both types of transport mechanisms play an important role. When the approximation of Bosanquet is required for modelling accurately. This regime is of interest for a high level of porous dielectric humidity sensors.

6.3 Molecular Diffusion Regime

As the pore size gets closer to 1000 nm, D_k is much greater than D_b . The diffusion process becomes more like the free-air diffusion process. The effective diffusion coefficient approaches the bulk diffusion coefficient.

7. TRANSPORT RESISTANCE ANALYSIS

The Bosanquet model can be explained by diffusion resistances. The overall transport resistance is:

$$R_t = R_m + R_k$$

R_m and R_k are molecular and Knudsen diffusion resistances (figure 5), respectively. Smaller pores can significantly affect Knudsen resistance. Knudsen resistance decreases as the dimensions of the pores are increased, and molecular diffusion takes over. This interpretation offers a helpful physical interpretation of the behavior of moisture

transport in porous materials. Conceptual Representation of Bosanquet Approximation as a

series combination of molecular and Knudsen Resistances is given in figure 5.

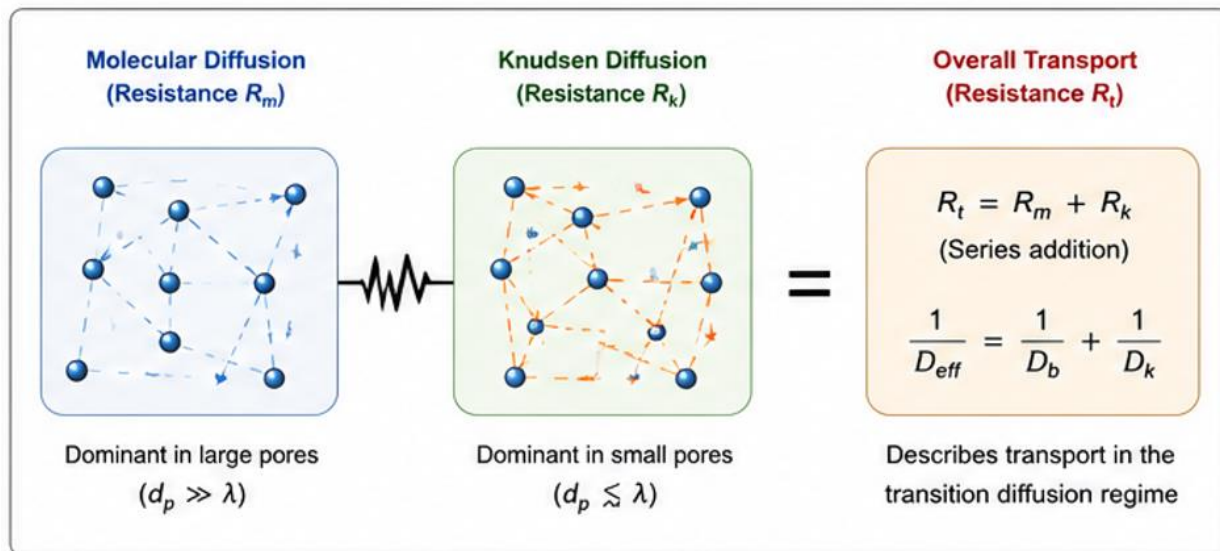


Figure 5: Conceptual Representation of Bosanquet Approximation as a series combination of molecular and Knudsen Resistances

9. OUTCOME AND SUGGESTIONS FOR HUMIDITY SENSOR DESIGN

Numerical analysis gives valuable information for the development of humidity sensors. Extremely small nanopores enhance the adsorption surface area but slow down the diffusion rate. The larger the pores, the better the diffusion transport, but the less adsorption area. A hierarchical pore structure, that combines diffusion efficiency with adsorption capacity, therefore ought to be incorporated in a sensor optimized to perform its function. These can be fast transportation channels as well as high adsorption points.

9. FUTURE EXTENSIONS

The Bosanquet approximation is able to provide coupled diffusion effects but more mechanisms are required for realistic sensor modeling. Additional future work should include:

- Adsorption-desorption kinetics
- Capillary condensation
- Surface diffusion
- Multi-scale pore networks
- SEM-derived pore distributions

All of these factors are likely to further enhance prediction accuracy of transient sensor behavior.

10. Relevance to Intelligent Sensing, Assistive Technologies, and Autonomous Systems

Accurate humidity sensing is increasingly important in intelligent environments, assistive technologies, healthcare monitoring systems, and autonomous robotic platforms. Modern robotic and cyber-physical systems often operate in dynamic environments where environmental conditions directly influence system reliability, user comfort, sensor calibration, and operational safety. Humidity monitoring is particularly relevant in healthcare facilities, assisted-living environments, smart homes, agricultural automation systems, and autonomous inspection platforms, where continuous environmental awareness is required.

The diffusion behavior analyzed in this study provides valuable insight into the design of humidity sensors capable of achieving improved response speed, sensitivity, and long-term stability. Understanding the transition between molecular diffusion and Knudsen diffusion enables the

optimization of porous dielectric structures for rapid moisture detection in resource-constrained sensing platforms. Such capabilities are important for distributed Internet-of-Things (IoT) sensor networks, wearable assistive devices, environmental monitoring systems, and robotic platforms that rely on accurate environmental perception.

Furthermore, the Bosanquet-based modeling framework provides a theoretical foundation for developing next-generation intelligent sensing systems in which environmental information can be integrated with machine learning and autonomous decision-making algorithms. Future research may explore the integration of optimized humidity sensors into robotic perception systems, smart assistive technologies, and autonomous monitoring applications requiring real-time environmental awareness and adaptive operation.

11. Future Research Directions

While the Bosanquet approximation provides a practical framework for modeling coupled molecular and Knudsen diffusion, several opportunities exist for extending the present work. Future studies should incorporate adsorption-desorption kinetics, capillary condensation, surface diffusion, and multi-scale pore-network models to achieve a more realistic representation of moisture transport in porous dielectric materials. Experimental validation using fabricated porous sensor structures and SEM-derived pore-size distributions would further improve model accuracy and applicability. In addition, transient diffusion behavior under varying temperature and humidity conditions should be investigated to better represent real operating environments. The integration of advanced numerical models with machine learning techniques may also enable predictive optimization of pore architectures for improved sensing performance. Such developments could support the design of next-generation humidity sensors for intelligent sensing systems, smart environments, healthcare monitoring, assistive technologies, Internet-of-Things platforms, and autonomous robotic applications requiring

reliable environmental awareness and adaptive decision-making.

12. Conclusion

This study presented a numerical investigation of moisture transport in porous dielectric materials using the Bosanquet approximation, which combines molecular and Knudsen diffusion into a unified transport model. Parametric analysis demonstrated that pore size strongly influences Knudsen diffusion, effective diffusion coefficients, and overall transport resistance. The results identified three distinct transport regimes: Knudsen-dominated diffusion in nanoscale pores, a transition regime where molecule-molecule and molecule-wall interactions contribute simultaneously, and molecular diffusion in larger pores. The Bosanquet approximation was shown to provide a smooth and physically meaningful description across these regimes without requiring separate diffusion models. The findings highlight the importance of pore geometry in determining moisture transport characteristics and provide useful guidance for the design of high-performance porous dielectric humidity sensors. Furthermore, the study establishes a theoretical foundation for future diffusion-adsorption modeling and the development of advanced sensing systems for intelligent environments, assistive technologies, and autonomous monitoring applications.

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