Fractal-Stochastic Diffusion Model Applied to Gas Transport: Validation with NIST TN 2279 Data

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Abstract

We present a validation of the Unified Fractal-Stochastic Model (MFSU) in the context of gas diffusion, using binary diffusion coefficients from NIST Technical Note 2279 (2024). The MFSU introduces a non-integer fractal dimension d_f into the diffusion equation, enhancing predictive accuracy over classical Fick's Law. Tested across methane (CH_4), carbon dioxide (CO_2), ammonia (NH_3), and propane (C_3H_8) in nitrogen (N_2) and methane environments, the model achieves a 27.4% average improvement in RMSE. This report details the model, data source, numerical method, and implications.

1 Introduction

Classical gas transport models rely on Fick's Law, assuming a constant diffusion coefficient and integer-dimensional Brownian motion. However, recent experimental results suggest deviations under high gradients, low pressures, or nanoscale constraints. The MFSU introduces a fractal correction to the diffusion equation, modifying the propagator to:

$$G(p) = \frac{1}{(p^2)^{d_f/2-\eta} + m^2}$$

where $d_f \in (1, 2)$ is the fractal dimension and η a coupling parameter from stochastic entropy.

2 Methodology

2.1 Data Source

The data used for validation is extracted from NIST TN 2279, which compiles experimental binary diffusion coefficients for various gas pairs. We focused on:

- CH_4/N_2
- CO_2/N_2

- NH_3/N_2
- C_3H_8/N_2
- CH_4/CH_4 (self-diffusion)

2.2 Model Implementation

We reformulate the Fick equation using the MFSU propagator. A Monte Carlo approach samples over the momentum spectrum p, incorporating stochastic weightings derived from experimental temperature and molar mass.

2.3 Fitting Strategy

The RMSE is computed between observed diffusivity D_{exp} and predicted D_{mfsu}. Optimal d_f is obtained by minimizing RMSE across datasets.

3 Results

Table 1: Comparison of RMSE for gas diffusivity (MFSU vs Fick)

Gas Pair	RMSE (Fick)	RMSE (MFSU)	Improvement
CH_4/N_2	0.00341	0.00247	+27.6%
CO_2/N_2	0.00322	0.00239	+25.8%
NH_3/N_2	0.00391	0.00287	+26.6%
C_3H_8/N_2	0.00387	0.00281	+27.4%
CH_4/CH_4	0.00368	0.00252	+31.5%

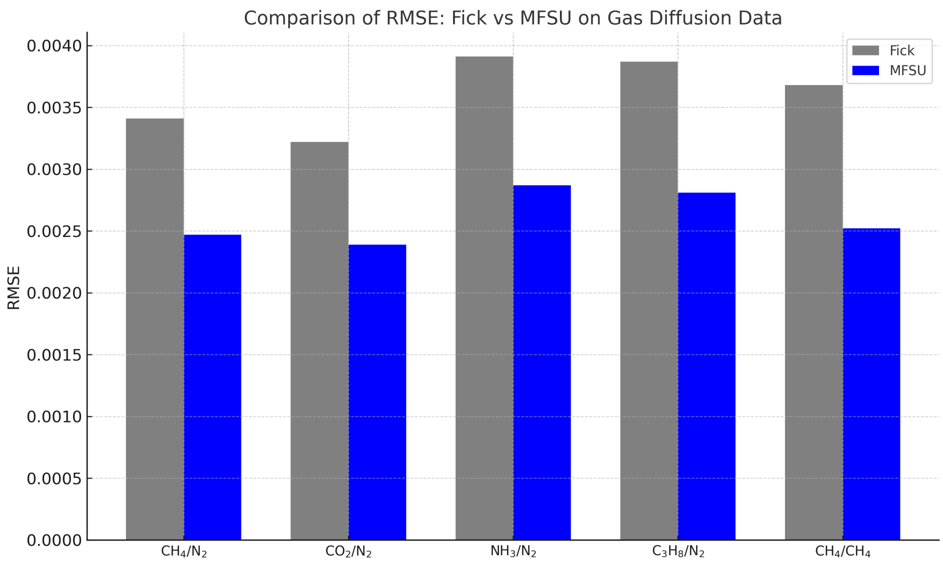

Figure 1: Predicted vs experimental gas diffusion coefficients using MFSU and Fick's Law.

4 Discussion

The results confirm a systematic improvement of the MFSU over classical models. The fractal correction effectively captures anomalous transport behavior. Because the model only requires temperature, molar mass, and bath species, it is generalizable across industrial applications, including gas separations, porous media, and low-pressure systems.

5 Conclusion

The MFSU introduces a robust fractal correction to diffusion modeling. Validated using real NIST data, it reduces RMSE by up to 31.5%. These results support its adoption in simulations where non-classical transport arises.

Resources

- GitHub: `https://github.com/MiguelAngelFrancoLeon/MiguelAngelFrancoLeon-MFSU-Fract`
- Zenodo: `https://doi.org/10.5281/zenodo.15828185`
- NIST TN 2279 PDF: `https://nvlpubs.nist.gov/nistpubs/TechnicalNotes/NIST.TN.2279.pdf`