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Investigation of Gas Diffusion by using Bout++ Fluid Simulation: Role of Density Gradient

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The present work simulate gas diffusion by fluid simulation and examine 1-D situation using BOUT++. We have extended the BOUT++ code to solve the gas diffusion fluid equations, added a simple neutral fluid model, created a mesh generator, and collected a set of complex test problems for diffusion codes. Progressing stepwise, firstly, the gas diffusion equation in 1-D, 2-D, and 3-D has been solved with the help of simulation and then added the convective term to the diffusion equation for its solution. The simulations showed that the convective term has a significant effect on the process of diffusion. Also, the diffusion coefficient that depends on the type of gas shows its influence on the diffusion process. For uncovering the role of density gradient, the initial density profile is taken to be Gaussian and then the results are compared with the case of super-Gaussian density profile. In the case of super-Gaussian density profile, the gas diffusion takes place at a much faster rate. The study puts a light on the basic diffusion process, playing role in the concept of particle acceleration and the study of Tokamaks for its application in nuclear fusion.

Keywords: Gas diffusion, Bout++, Fluid simulation, Super-Gaussian density profile

1 Introduction

The diffusion is defined as the net movement of atoms, ions, molecules etc. from higher concentration to lower concentration region. The study of gas diffusion plays an important role in particle diffusion in physics. The diffusion is also effectively used in chemistry, biology, and other fields of science, explaining different kinds of phenomena such as cell interactions with biological metamaterials[1], heat diffusion leading to stresses in energy generation systems[2-3] and combat aircraft[4-5]. In general, this is understood that a gradient in chemical potential or Gibbs free energy drives the diffusion. The interesting property that makes the study of diffusion so fascinating is that it does not require the bulk motion but depends on the particle random walk[6].

In metal-organic frameworks, the diffusion of gases is an important property in measuring the suitability of a material for industrial surface assimilation or partition applications[7]. In the metal-organic framework, many classical simulation and experimental studies have been focused on the transport properties of industrially useful gases such as H_2, CH_4, CO_2 [8-12]. The diffusion coefficients of high-temperature gases and gas mixtures are important inputs in numerical simulations of plasma phenomena. In this direction, diffusion coefficients of nitrogen, oxygen, argon, mixtures of argon and nitrogen, and mixtures of argon and oxygen, have been calculated[13]. Not only this, an emphasis has been put on the basic diffusion process focusing on its role in the concept of particle acceleration and the study of Tokamaks for its application in nuclear fusion[14]. The diffusion of nitrogen molecules in low carbon steels have led to hardening of surface, which is quite useful in automobile industry[15,16]. Here, this is important to understand the formation of sheath and its properties such as thickness and potential variation[17-20].The potential variation in plasmas has also been found to support the soliton evolution during laser interaction[21, 22]. On the other hand, diffusion of radon gas through thermocol sheet has been investigated keeping in mind that the long exposure to indoor radioactive gases increases the risk of health-related issues[23]. Analytical study has been conducted to see the effect of heat and mass transfer of a MHD Casson fluid flow over an inclined layer[24]. Numerical simulations have been performed to study blood flow of Casson fluid considering Brownian motion and thermophoresis effect[25].

For investigating the above systems, generally[26] the second-order central differencing method is applied for the first derivative $\frac{d}{dx}$ and the second derivative$\frac{d^2}{dx^2}$. The BOUT++ is a 3-D nonlinear finite-difference fluid simulation code for solving general systems of Partial Differential Equations[27, 28]. Recently, higher end

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*Corresponding author: E-mail: gauravkmr909@gmail.com simulations have also been performed for solving equations governing the temperature gradient driven folding of cumbersome structures[29]. In the present work, we have developed a simulation model of gas diffusion by employing a one-dimensional fluid simulation for high-temperature nitrogen and oxygen gases. After this, we have extended the code in Bout++ for two-dimensional and three-dimensional situations. Specifically, we have solved the gas diffusion equation in 1-D, 2-D, and 3-D with the help of simulation by adding the convective term to the diffusion equation. Finally, we observed the role of the density gradient by considering the initial density profile to be Gaussian and super-Gaussian and comparing the results of these two cases.

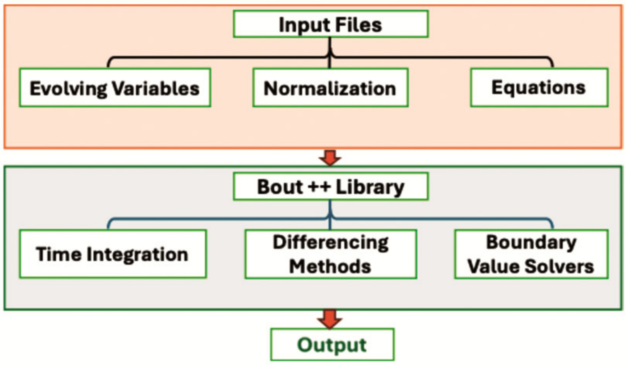

Fig. 1 — Schematic of Bout++ simulation method

2 Simulation Setup and Basic Equations

Recently numerical methods have been applied to solve the coupled equations for obtaining ion-density-driven thrust[30-33]. Random Walk Simulations have been applied to investigate the effective transport properties of Carbon Cloth gas diffusion layers[34]. However, the problem of gas diffusion in the present work has been simulated with the help of Bout ++ software, which is a fluid simulation parallel code and whose schematic is shown in Fig. 1. The simulation box is three dimensional with $x = 104$, $y = 100$, and $z = 100$, respectively, and the step size is $dx = 1$, $dy = 1$, and $dz = 1$. The number density of gas $n = 10^{10} / m^3$.Here we solve 3-D gas diffusion Eq 1 with the initial density profile as Gaussian[35]. In the equation, the symbol D represents the diffusion coefficient. In the case of convective diffusion, we solve Eq 2 by using Bout ++ and putting the convective term multiplier constant as 0.9. The output data is diagonalized with the help of python software.

$$\frac{\partial \mathrm{n}}{\partial \mathrm{t}} = \mathrm{D}\left[\frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} + \frac{\partial^2 n}{\partial z^2}\right] \qquad \ldots (1)$$

$$\frac{\partial n}{\partial t} = D\left[\frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} + \frac{\partial^2 n}{\partial z^2}\right] - 0.9\frac{\partial n}{\partial x} \qquad \ldots (2)$$

3 Results

In the first case, nitrogen gas with diffusion coefficient D = 0.010 m^2/s is considered[13, 36, 37] and simulated through Eq 1 taking the initial density profile as Gaussian. The obtained results are shown in Fig. 2. A

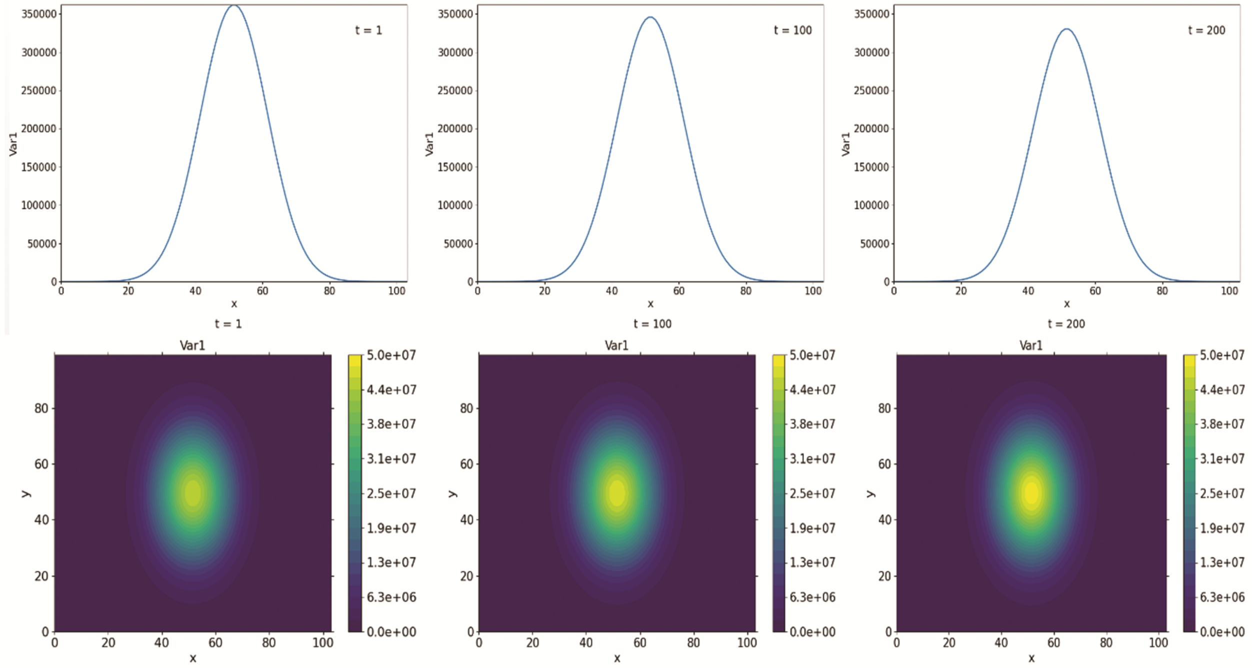

Fig. 2 — Density at different times for the diffusion of nitrogen gas in 1-D (upper) and 2-D (lower) simulations

comparison of all the graphs shows a reduction in the density of gas with a sharp almost Gaussian peak with advancing time. This is due to the density reduction in the y-z plane and enhancement in the x-z plane. This can be said that the positive diffusion occurs in 2-D case, but it appears to be negative when one does not consider the second dimension. In the second case, the diffusion of oxygen gas is investigated through in Fig. 3 where we have taken $\mathrm{D} = 0.018\,\mathrm{m}^2/\mathrm{s}$in Eq 1. A faster diffusion of oxygen is observed, which can be seen through the reduction in peak. This happens due to the larger diffusion coefficient of oxygen.

Actually, the simulation was run for 3-D situation considering x-, y- and z-variations. However, the variation of density was shown in 2-D case (variation in x-y plane). Now we have included Fig. 4 that shows the variation in x-z plane as well. This is seen that the density variation is not so great in this plane, rather it shows dominant variation in the x-y plane.

In the third case on adding the connective term in the x-direction ($0.9dn/dx$) in Eq 1, movement of the Gaussian peak in the x-direction is observed Fig. 5. In the last case, we have considered the initial density to be the super-Gaussian[38, 39], and the results are shown in Fig. 6 the super Gaussian profile is chosen to investigate the role of density gradient in the process of gas diffusions. A comparison of Figs. 5 and 6 reveal much faster diffusion of the gas in the case of

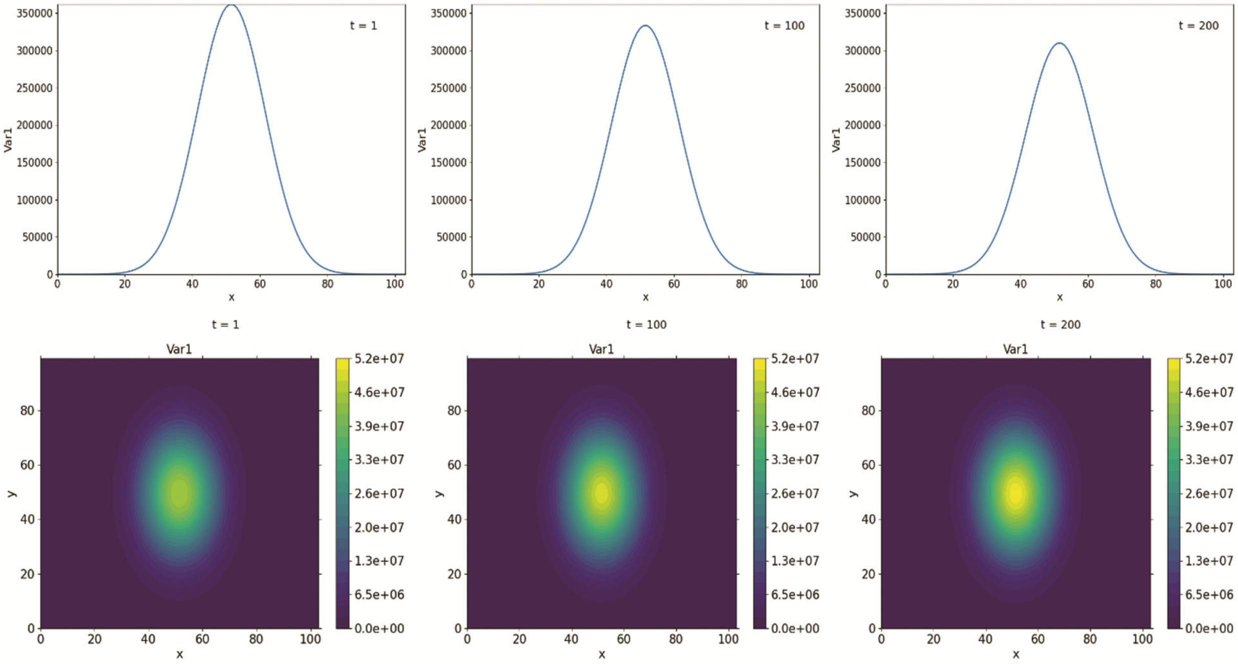

Fig. 3 — Density at different times for the diffusion of oxygen gas in 1-D (upper) and 2-D (lower) simulations

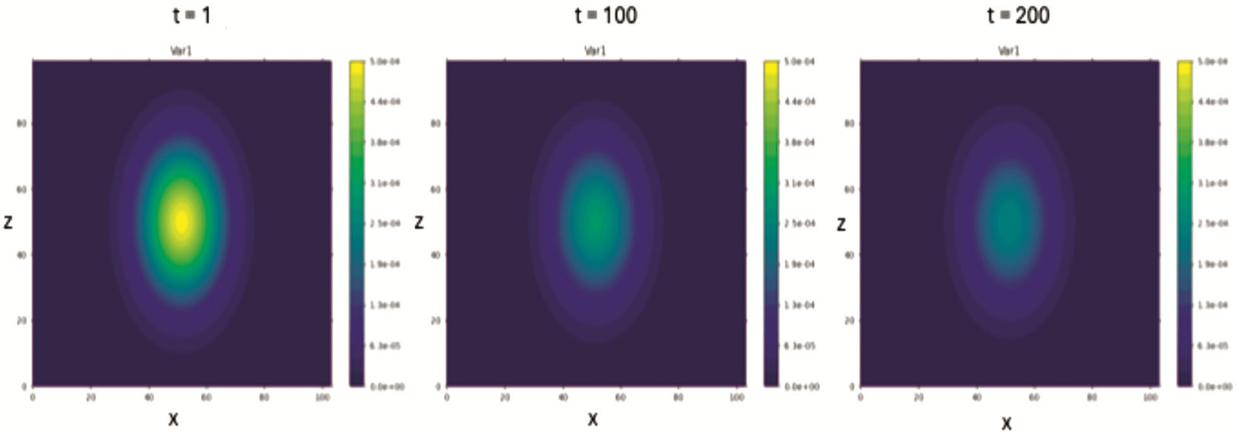

Fig. 4 — Density at different times for the diffusion of oxygen gas in 2-D (x-z plane) simulations

super-Gaussian profile of the initial density, i.e. when there is a larger gradient in the density. Since the faster diffusion also occurred in the case Figs. 2 and 3 of gas carrying higher diffusion coefficients, we can say that the role of density gradient in the density is similar to the enhanced diffusion coefficient.

The impact of higher density gradient on the gas diffusion process can be further understood when we select the initial density profile to be the super-Gaussian with different orders. Hence, in Figs. 7 and 8 we have shown the gas density diffusion with different order of p super-Gaussian profile, It is clearly appearing in these

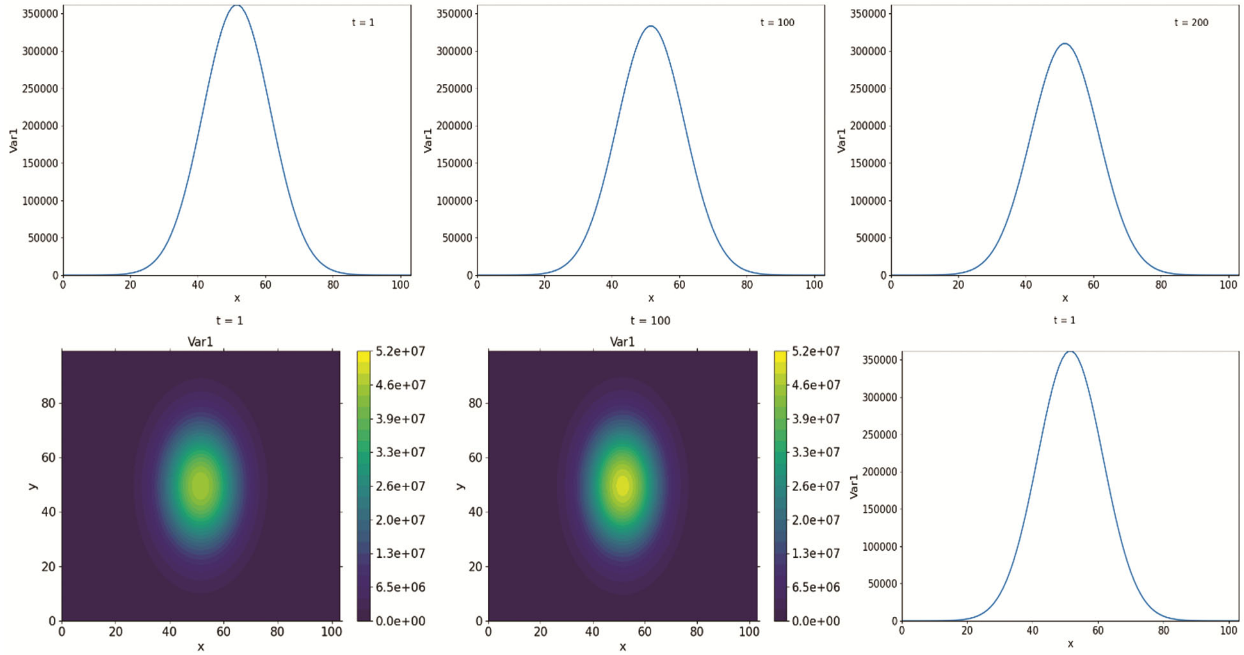

Fig. 5 — Convective diffusion of density (Gaussian profile) at different times in 1-D (upper) and 2-D (lower)

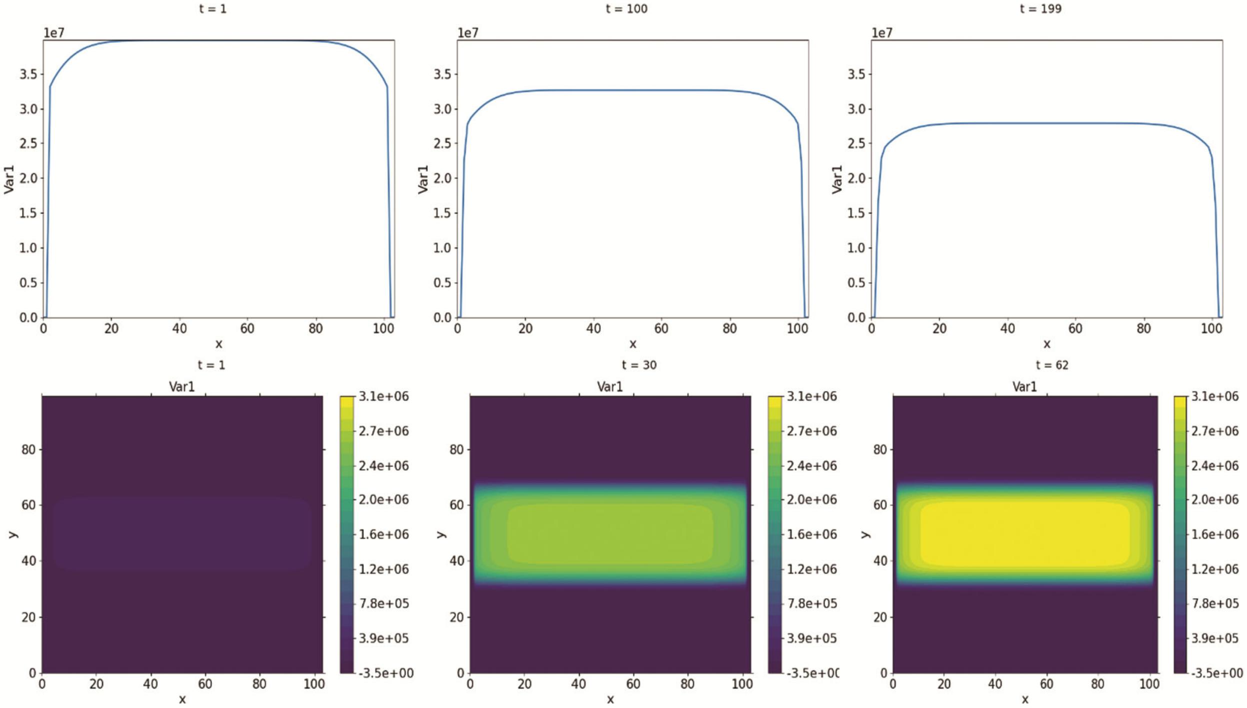

Fig. 6 — Convective diffusion of density (super-Gaussian profile) at different times in 1-D (upper) and 2-D (lower) simulations

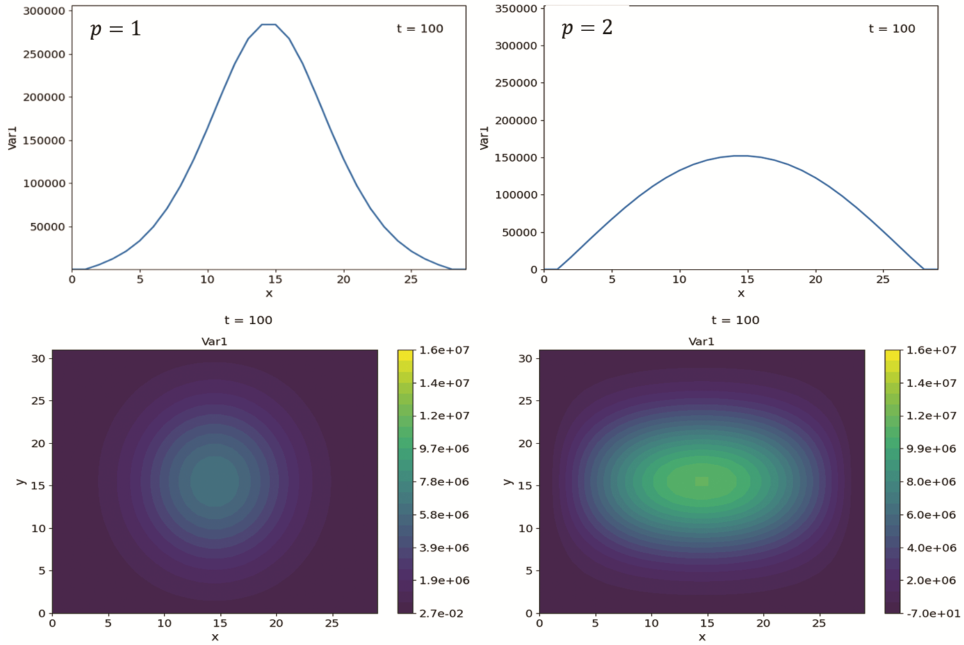

Fig. 7 — Diffusion of Super-Gaussian density profile at same times with order$p = 1$ and$p = 2$ in 1-D (upper) and 2-D (lower) simulations

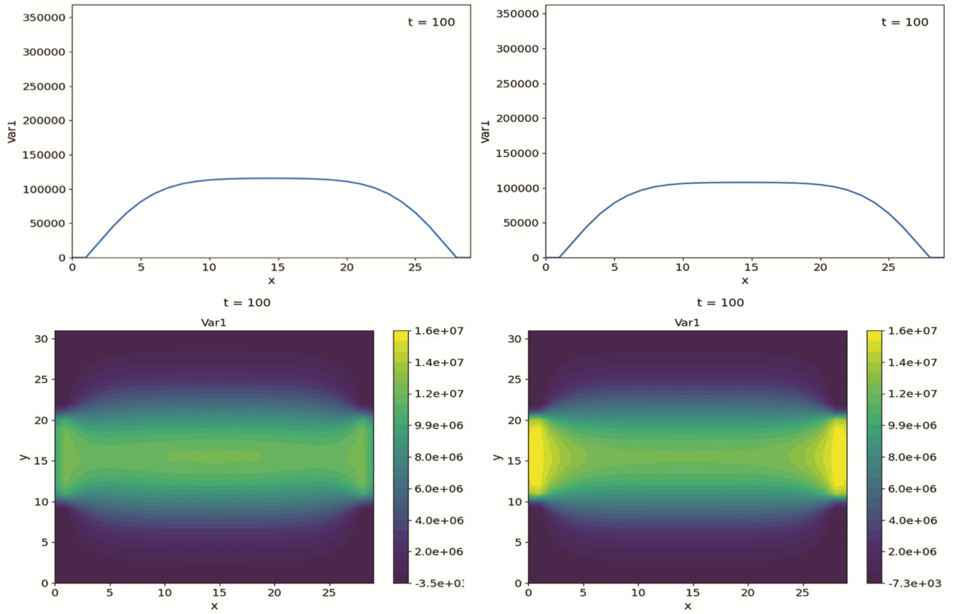

Fig. 8 — Diffusion of Super-Gaussian density profile at same times with order s$p = 4$ and $p = 6$ in 1-D (upper) and 2-D (lower) simulations

figures that if the order of super-Gaussian profile increases then the diffusion rate becomes much faster. In 1-D (upper) simulations, i.e. in Fig. 7 it is seen that at the same time ($t = 100$) and at the second order ($p = 2$) the diffusion is faster compared to the case with $p = 1$ Gaussian. The increased diffusion super-Gaussian of the gas is further observed with the increase in the order of super-Gaussian profile, i.e. $p = 4\ to\ p = 6$ in Fig. 8.

The diffusion process studied in the present article will have applications to gas sensitive nanostructure sensor[40], mapping the variation in indoor radon[41] and transient natural convection magneto hydrodynamic motion[42].

4 Conclusion

The diffusion coefficient of gas that depends on the type of gas shows its influence on the diffusion process.

The simulations showed that the diffusion coefficient and the convective term have a significant effect on the process of diffusion. In the case of nitrogen gas, the gas density diffuses at the rate $0.01/m^3s$ and in the case of oxygen gas, the rate is $0.018/m^3s$, when the initial density profile is taken as Gaussian. However, in the case of super-Gaussian density profile the gas density diffuses at a faster rate of 0.08 $/m^3s$. These rates remain the same when we consider the convective term in the equations. In conclusion, the gas diffusion takes place at a much faster rate in the case of initial density profile as the super-Gaussian profile, inferring that the gases having gradient in their densities diffuse faster than the gases having uniform density. Also, the role of the density gradient is found to be similar as that of the increased diffusion coefficient.

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