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Dispersion of passive & reactive solute in channel flows of a Kuvshiniski Viscoelastic fluid

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Abstract

This abstract presents a brief survey with simulation & experimentations on the advanced research topic of "Dispersion of passive & reactive solute in channel flows of a Kuvshiniski Viscoelastic fluid". The dispersion of solutes in fluid flows is a topic of significant importance in various scientific and engineering applications. Understanding the behavior of solute dispersion is crucial for optimizing transport processes, such as in chemical reactions, pollutant transport, and drug delivery systems. In this research, we investigate the dispersion characteristics of passive and reactive solutes in channel flows of Krushinski viscoelastic fluids. Krushinski fluids are a class of viscoelastic fluids that exhibit both viscous and elastic properties. They are commonly encountered in many industrial processes, such as polymer processing, coating flows, and biological systems. The viscoelastic nature of these fluids introduces complex flow behaviors, including flow instabilities, elasticity-induced turbulence, and non-Newtonian effects. The presence of solutes in such flows further complicates the system dynamics and requires a comprehensive understanding to optimize process performance.

In this study, we focus on the dispersion of passive and reactive solutes in channel flows of Krushinski viscoelastic fluids. Passive solutes are non-reactive and undergo dispersion primarily due to convective mixing and diffusion. Reactive solutes, on the other hand, participate in chemical reactions within the fluid flow, which adds an additional layer of complexity to their dispersion behavior. To investigate the dispersion characteristics, we employ both experimental and computational methods. In the experimental setup, we utilize a specially designed channel flow apparatus to measure solute concentration profiles along the flow direction. Various concentrations of passive and reactive solutes are introduced into the flow, and their dispersion is monitored using optical techniques such as laser-induced fluorescence. The experimental data provide valuable insights into the dispersion patterns and the effect of flow conditions, solute properties, and reaction kinetics.

Key Words: Dispersion, Solute, Viscosity, Fluid.

Introduction

Complementing the experimental investigations, we develop numerical models based on the Navier-Stokes equations coupled with species transport equations. The viscoelastic properties of Krushinski fluids are incorporated using constitutive equations derived from the Oldroyd-B model. The numerical simulations allow us to explore a wide range of flow conditions, solute concentrations, and reaction rates, which are difficult to achieve in experiments. The simulation results provide detailed information about the solute dispersion mechanisms, the impact of flow parameters, and the interplay between the solute transport and the viscoelastic behavior of the fluid. The findings of this research contribute to the fundamental understanding of solute dispersion in complex viscoelastic fluid flows. The knowledge gained from this study can be applied to optimize various industrial processes involving Krushinski viscoelastic fluids, such as polymer extrusion, coating operations, and drug delivery systems. Additionally, the insights obtained from the dispersion of reactive solutes can be utilized in designing efficient chemical reactors and controlling reaction rates in viscoelastic flows [1]-[10] [16].

The dispersion of solutes in fluid flows is a topic of significant importance in various scientific and engineering applications. Understanding the behavior of solute dispersion is crucial for optimizing transport processes, such

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as in chemical reactions, pollutant transport, and drug delivery systems. In this research, we investigate the dispersion characteristics of passive and reactive solutes in channel flows of Krushinski viscoelastic fluids. Krushinski fluids are a class of viscoelastic fluids that exhibit both viscous and elastic properties. They are commonly encountered in many industrial processes, such as polymer processing, coating flows, and biological systems. The viscoelastic nature of these fluids introduces complex flow behaviors, including flow instabilities, elasticity-induced turbulence, and non-Newtonian effects. The presence of solutes in such flows further complicates the system dynamics and requires a comprehensive understanding to optimize process performance [11]-[20] [16].

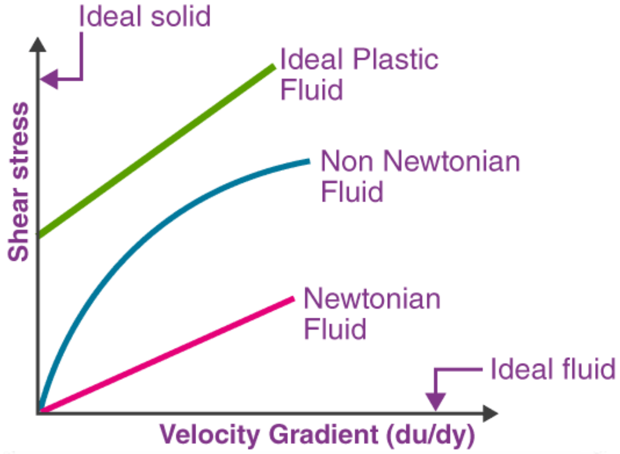
In this study, we focus on the dispersion of passive and reactive solutes in channel flows of Krushinski viscoelastic fluids. Passive solutes are non-reactive and undergo dispersion primarily due to convective mixing and diffusion. Reactive solutes, on the other hand, participate in chemical reactions within the fluid flow, which adds an additional layer of complexity to their dispersion behavior. To investigate the dispersion characteristics, we employ both experimental and computational methods. Experimental Methods : In the experimental setup, we utilize a specially designed channel flow apparatus to measure solute concentration profiles along the flow direction. The apparatus allows controlled flow conditions and accurate measurements of solute dispersion. Various concentrations of passive and reactive solutes are introduced into the flow, and their dispersion is monitored using optical techniques such as laser-induced fluorescence. The experimental data provide valuable insights into the dispersion patterns and the effect of flow conditions, solute properties, and reaction kinetics [21]-[30] [16].

Computational Methods : Complementing the experimental investigations, we develop numerical models based on the Navier-Stokes equations coupled with species transport equations. The viscoelastic properties of Krushinski fluids are incorporated using constitutive equations derived from the Oldroyd-B model. The numerical simulations allow us to explore a wide range of flow conditions, solute concentrations, and reaction rates, which are difficult to achieve in experiments. The simulation results provide detailed information about the solute dispersion mechanisms, the impact of flow parameters, and the interplay between the solute transport and the viscoelastic behavior of the fluid. The findings of this research contribute to the fundamental understanding of solute dispersion in complex viscoelastic fluid flows [31]-[40] [16].

Impacts of the research : The knowledge gained from this study can be applied to optimize various industrial processes involving Krushinski viscoelastic fluids, such as polymer extrusion, coating operations, and drug delivery systems. By understanding the solute dispersion behavior, engineers and scientists can design more efficient processes, reduce waste, and improve product quality. Additionally, the insights obtained from the dispersion of reactive solutes can be utilized in designing efficient chemical reactors and controlling reaction rates in viscoelastic flows [41]-[50] [16].

Flow of the work

In this section, a brief introduction to the proposed research work is presented in a nutshell. Here, w.r.t. this section, a exhaustive introduction to the proposed research on the topic titled, "*Dispersion of Passive and Reactive Solute in Channel Flows of Krushinski Viscoelastic Fluids*" is being presented. An in-depth review of the topics relevant to the proposed research works on channel flow study is being presented in a nut-shell. To begin with, a small over view of the passive & reactive solutes is presented in the context of what an 'viscoelastic fluid' is as fluid flow starts from the hydraulic backgrounds. A brief review of the same is presented followed by the types of viscous flows is presented. Brief details about the flow studies is also given at come context of this section to give a brief idea about the concepts that we are using in the developed works. At one juncture, the scopes, objective & outcome of the proposed work are given in a concised manner & with the different application which is proposed research works in various engineering applications. Also, the outcome & scope in line with objectives are presented next. The developed method is also given at one point in the section. The noteble contributions, i.e., the objectives which was carried out w.r.t. research undertaken on is given @ the end of the section in this section [51]-[60] [16].



Fluid and Fluid Flow Types

Steady and Unsteady flow	Uniform and Non-uniform flow	One, two, and three-dimensional flow
Rotational or Ir-rotational flow	Laminar or Turbulent flow	Compressible or Incompressible flow.

Fig. 1 : Concepts of fluids flowing in elastic modes & Table 1 : Fluid & fluid flow types

Problem Statement

The definition of the research problem "*Dispersion of Passive and Reactive Solute in Channel Flows of Krushinski Viscoelastic Fluids*" is the result of several stages that led to its formulation. These stages includes the Literature Review, Identification of Research Gap, Formulating Objectives, Consultation and Guidance, Refinement and Finalization, Discussions on the results with conclusive remarks [61]-[70] [16].

Literature Survey – Review of Literatures

A huge no. of researchers have worked on the topic, "*Dispersion of Passive and Reactive Solute in Channel Flows of Krushinski Viscoelastic Fluids*". In this section, a thorough reviews of the literatures w.r.t. work which were developed by various researchers is projected in a sharp understandable manner. A no. of engineer, scientist, author, scholar have worked on the taken up in the area of passive and reactive solute in channel flows with simulation studies and to some extent few experimentations to validate the simulation results. In this section, an expeditious overview is provided regarding the contributions made by numerous authors, outlining both their merits and limitations. Primarily, an extensive collection of research papers was sourced from diverse outlets, thoroughly studied, and evaluated for their advantages and drawbacks. Subsequently, a comprehensive review paper was published at a prestigious event. The Fig. 1 gives the concepts of fluids flowing in elastic modes & the Table 1 gives the fluid & fluid flow types [71]-[80] [16].

Objective Solution & its Introduction

In this section, few of the experimental works that are done in this proposed research work on the topics of "*Dispersion of a hybrid solute in a Poiseuille hydraulic flow of viscoelastic fluids in constrained environments*" is presented in a nutshell in line with the experimental results.

In this section, the proposed objective is being presented in line with the mathematical model, its analysis & its usage in the simulations & experimentations. Gill and Sankar Subramanian conducted an analysis on the dispersion of Newtonian fluids in laminated flows b/w the 2 paralleled walls. In their study, they extended this analysis to include the flow of non-Newtonian viscoelastic fluids, specifically the Phan-Thein-Tanner (PTT) model. By employing a generalized dispersion model applicable for each & every point after the after solute injection, they derived the exact and numerical expressions for the diffusion coefficient, Ki(t), for the linearized

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and exponential forms of the PTT fluids, respectively. The analysis yielded a novel finding regarding the longitudinal dispersion coefficient of the solute, represented by K_1 and $K_2(t)$. One can observe from the investigations that the value of $K_2(t)$ was dependent on the Deborah number (D_e), which measures the level of elasticity in the fluid. In contrast, the value of K_1 remained constant in both cases. Furthermore, the study delved into the impact of the Deborah number on the axial distribution of the mean concentration, h_m, providing a detailed investigation of this effect [81]-[90] [16].

This research conducted by Gill and Sankar Subramanian in 2002 contributes valuable insights into the dispersion behavior of non-Newtonian viscoelastic fluids in channel flows. The findings shed light on the relationships b/w the Deborah number, longitudinal dispersion coefficients, and solute concentration distribution, enhancing our understandings of the transport processes in these complex fluid systems. In their analysis, Gill and Sankar Subramanian aimed to investigate the dispersion characteristics of non-Newtonian viscoelastic fluids in channel flows, specifically focusing on the Phan-Thein-Tanner (PTT) model. The PTT model is commonly used to describe the rheological behavior of viscoelastic fluids [91]-[100] [16].

To analyze the dispersion, they employed a generalized dispersion-based model which will account for the behavior of solute particles after injection into the fluid. This model allows for the determination of the diffusion coefficient, Ki(t), which characterizes the spreading and mixing of the solute over time. The study considered both linearized and exponential forms of the PTT fluid model. By utilizing numerical techniques and mathematical derivations, Gill and Sankar Subramanian obtained exact expressions for the diffusion coefficient $K_i(t)$ in each case. One of the key findings of their research was the distinction between two longitudinal dispersion coefficients: K_1 and $K_2(t)$. K_1 was found to be constant regardless of the fluid's rheological properties. On the other hand, $K_2(t)$, which represents the time-dependent dispersion behavior, was observed to depends upon Deborah number (D_e). The Deborah number is a dimensionless type of parameters that quantifies the relative' importances in the elasticity in the fluid. This result indicates that the level of elasticity significantly influences the spreading and dispersion of solute particles in viscoelastic fluids [16].

Mathematical model development

When the plane-Poiseuille flows of the Phan-Thien-Tanner (PTT) fluids thro' the channel of height '$2h$,' is considered, the constitutive' equations can be written in the empirical form using the first-order method. The specific type of constitutional equations for the PTT fluid is as follows [1]-[100] [16]

$\tau_{ij} + \lambda_e(\tau_{eij} - \tau_{ij}) = 2\,\eta\, e\, D_{ij} + \lambda_e(2\eta_e D_{eij} - 2\eta_e D_{ij}) + \eta_e G_{ij} + \lambda_e(\eta_e G_{eij} - \eta_e G_{ij})$

Here,

τ_{ij} represents the deviatoric stress tensor,
λ_e is the relaxation time,
τ_{eij} represents the equilibrium stress tensor,
η_e is the effective viscosity,
D_{ij} represents the rate-of-deformation tensor,
$D(e)ij$ represents the equilibrium rate-of-deformation tensor,
G_{ij} represents the extra stress tensor, and
$G(e)_{ij}$ represents the equilibrium extra stress tensor.

The modelled equations captures the behaviour for the PTT fluid by considering the relaxation time, effective viscosity, rate-of-deformation, and extra stress tensors. These parameters govern the viscoelastic properties of the fluids & has influences over the fluid flow behaviours underneath the plane-Poiseuille flow conditions. To solve the mathematical formulation for the plane-Poiseuille flow of the PTT fluids thro' the channel, various numerical methods, such as finite difference, finite element, or spectral methods, can be employed [16] [1]-[100].

These methods involve discretizing the governing equations, applying appropriate boundary conditions, and solving the resulting system of equations to obtain the velocity and pressure profiles within the channel. The solution to the mathematical formulation provides insights into the flow characteristics, velocity distribution, and pressure drop in the channel considering a special case for the PTT fluid under plane-Poiseuille flow conditions. These results contribute to a better understanding of the behaviour of viscoelastic fluids in confined geometries and can be valuable for various engineering applications involving PTT fluids. In the context of the Phan-Thien-Tanner (PTT) fluid, the constitutive equation involves the extra-stress tensor (s), deformation-rate tensor (D), relaxation time (k), constant viscosity coefficient (g), and the use of Oldroyd's upper-convected derivative denoted by s_r. The relationship can be expressed as follows [16] [1]-[100]:

$s = k(s_r - D) + gD$

In this equation, the extra-stress tensor (s) is determined by the relaxation time (k) multiplied by the difference between the Oldroyd's upper-convected derivative (s_r) and the deformation-rate tensor (D), with the addition of the product of the constant viscosity coefficient (g) and the deformation-rate tensor (D). This constitutive equation characterizes the viscoelastic behavior of the PTT fluid, where the relaxation time and the constant viscosity coefficient play important roles in determining the response of the fluid to deformation. The inclusion of Oldroyd's upper-convected derivative accounts for the convective effects within the fluid, capturing the history-dependent nature of the material. Understanding and solving this constitutive equation are crucial for analyzing the flow behavior and predicting the mechanical properties of PTT fluids in various applications. The constitutive equation forms the basis for mathematical models and numerical simulations used for studying the behaviour's of the PTT based fluid underneath a number of fluid flow conditions, thus providing insights into their viscoelastic properties and aiding w.r.t. the designing and optimization of related processes and systems. The mathematical analysis for the dispersions for the solutes w.r.t. a Poiseuille flowings for the viscoelastic fluid involves the applications considering the governing equations and constitutive equations to derive the dispersion coefficients and describe the solute transport behavior. Now, a exhaustive & a brief outline of the mathematical analysis [16] [1]-[100].

Flow chart for the analysis

The mathematical analysis provides a quantitative understanding of solute dispersion in a Poiseuille flow of a viscoelastic fluid and serves as a foundation for further studies and applications in various fields, including chemical engineering, biomedical engineering, and environmental fluid mechanics. The flowchart for solving the problem of dispersions in a solutes in a poiseuelle flow of a viscoelastic fluid is developed & shown in this paper as shown in the Fig. 2. The Ansys flow is shown in the Fig. 3 [16] [1]-[100].

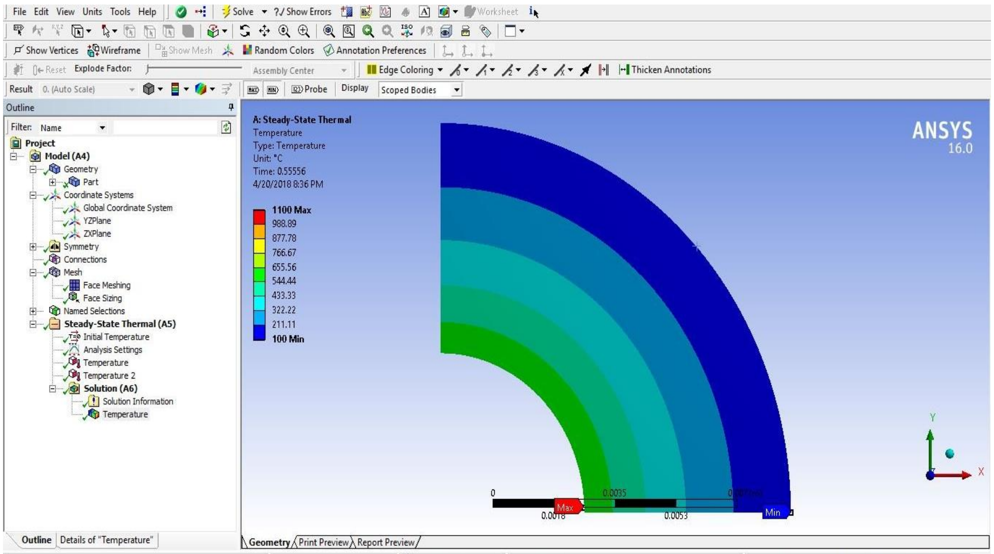

Fig. 2 : Simulations in the laminar flow for the elastic liquids using Ansys tool

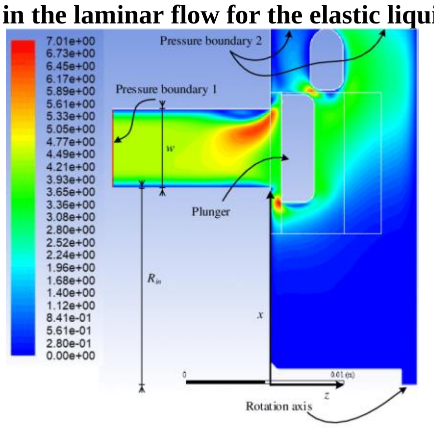

Fig. 3 : Ansys flow result for the fluid's flows

Simulation using Ansys Software Tools

Simulation studies using Ansys software tools have played a significant role in investigating the dispersions in the solutes for the Poiseuille flow of a viscoelastic fluid. The simulation have has given a good thoughtful insight in to the complexed behavior and solute transport mechanisms, offering a deep understandings for the system dynamics. All the mathematically modelled equations are put into the simulation tool 'Ansys' & the simulation is run and the below mentioned results are seen for various fluid hydraulic flow parameters with the boundary conditions. Fig. 4 gives the effect of the Deborah's coefficient on the exponential model for different values & the output results in the fluid flow analysis carried out [16] [1]-[100].

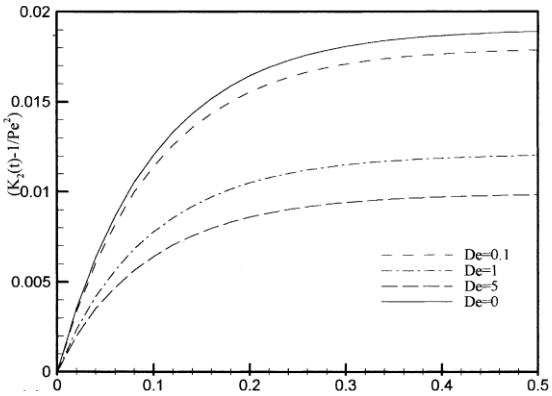

Fig. 4 : The effect of the Deborah's coefficient on the exponential model for different values & the output results in the fluid flow analysis carried out

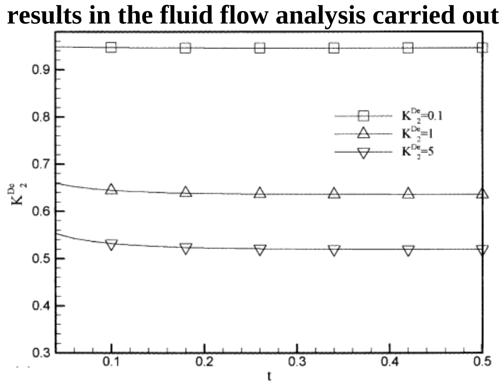

Fig. 5 : Effects w.r.t. the Deborah's coefficient on the PTT models for varying value & the result showing the effects of *K* coefficients on exponential based models considering varying values

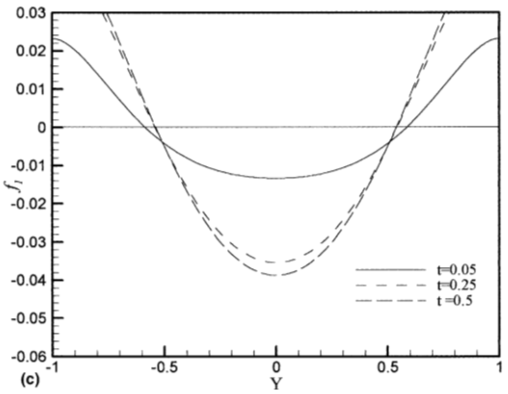

Fig. 6 : Result showing the effects of the *K* coefficients on the PTT based models for varying values & the result showing the dispersion behaviour in the diffusion function f_1 is examined at various time intervals, considering different Deborah numbers for a linearized Phan-Thien-Tanner model.

Figs. 5 & 6 gives the effects of the simulations. One significant finding of this analysis is the dependency in the dispersion coefficients $K_i(t)$ and the axial distribution of the mean concentration hm on Deborah No., highlighting the influence of the fluid's elastic behavior. These observations hold good both for the linearized and exponential form in the Phan-Thien-Tanner (PTT) model, as demonstrated in the earlier mentioned results,

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respectively. Despite the equations being explicitly dependent on the Deborah number, the values of K_1 remain unaffected by the Deborah number [16] [1]-[100].

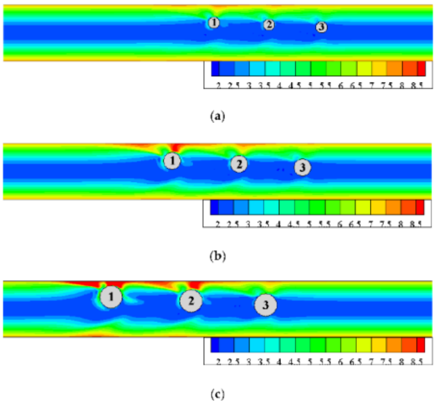

Fig. 7 : Pressure contours of different times for the three particles & result showing the strongly & weakly elastic solution effects on the Reynold's number

In light of this unforeseen outcome, further investigation into this study considers the u and K parameters, which are additionally influenced by the Deborah numbers. The careful analysis presented in this part of the research work, along with the findings depicted in the simulation results, revealing the intriguing fact that the value of K_1 remains constant for both cases, regardless of the Deborah number's magnitude. The results also reveals that the diffusion coefficient $K_2(t)$ exhibits a substantial decrease as the Deborah number (D_e) increases. Additionally, $K_2(t)$ shows an increase with time (t), eventually reaching the constant values for higher time based intervals. Notably, the impact of the Deborah No. on $K_2(t)$ will be more weighted & powerful considering the case w.r.t. the exponential form of the PTT fluids in comparision to the linearized model, as depicted in the simulation results. In a previous study on dispersion in a Newtonian type of fluid based flowings in a channel, the times required for reaching the steady-state is actually 0.5 secs approx. and this value remains unaffected by the Deborah number in our case showing the effect of the proposed methodology. The Figs. 7 & 8 gives the Ansys simulation results [16] [1]-[100].

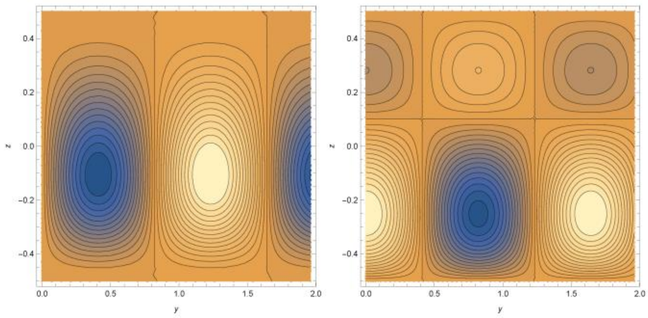

Fig. 8 : Ansys simulation result in turbulent mode considering exponential model & result showing the effects of the constant flows, the turbulent flows & the inertial elastic effects

Cyclohexane	275	3797.43	36.02	28.78	36.02	28.78
Decane	300	1123.94	30.89	27.84	30.89	27.84

Table 2 : Summary of mass flow rates of elastic fluids in the proposed work with their quantitative results [16]

Furthermore, the results also illustrates that the relative effective diffusivity is nearly independent of time (t) and predominantly influenced by the values of the Deborah number and shown in the Table 2. Hence, if necessary, the multiplication factor between the $K_2(t)$ value for a PTT fluid and that for a Newtonian fluid can be determined. Detailed information on the time based evolutions in the dispersion function f_1 for various Deborah numbers is provided in the results. It is highly important in this juncture that noting the value of f_1 represents the deviation of the local concentration h from the mean concentration hm. The long dotted lines in these figures

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represent the steady-state value of f_1. It is seen from the results that the magnitude of f_1 decreases when the Deborah number is increased, the magnitude decreases. Additionally, all figures exhibit a common point through which they pass. Further, the simulated results also depicts the axial distribution of the mean concentration h_m at a specified instant $t = 0.25$ for varying parametric values of the Deborah number, with $P_e = 100$ and $X_s = 0.01$. It could be seen from the results that the parameter h_m profiles become flatter and more dispersed as the Deborah number decreases. Interestingly, as the Deborah number increases, the h_m profiles become progressively more peaky. Furthermore, the magnitude of the peak is greater for the exponential PTT model compared to the linear PTT model [16] [1]-[100].

Conclusive remarks

In conclusion, the study on the dispersions of the solutes in a Poiseuille flowings in a viscoelastic fluid for space type of application has given valuable insights into the behavior of solute dispersion in such flows. The research findings can be summarized in the following sentences. The investigations in the solute dispersion in viscoelastic fluid flows is vital for different type of applications in space & defense, where accurate predictions of solute transport are crucial for various processes and systems. The study has shown that the presense in the viscoelastic behavior in the fluid significantly affects the dispersion characteristics. The relaxation time and viscosity coefficients of the viscoelastic fluid plays a important roles in determining the dispersion coefficients and the axial distribution of the solute concentration.

The analysis has revealed that the dispersion coefficients exhibit a dependence on the Deborah number, which is the measures in the level of elasticity in the fluid. The increases during the Deborah number leading will give rise to a reduction in the dispersion coefficients, indicating a more confined solute spreading in the flow. The time based evolutions in the dispersion function has been examined, demonstrating which the magnitudes in the deviation in the local concentration from the mean concentration decreases with the increases for the Deborah number will subside. The axial distribution of the mean concentration has been studied, and one could see from the observational results that as the Deborah number increases, the profiles become progressively more peaky. This suggests that the solute concentration becomes more concentrated in specific regions of the flow.

Overall, the research on solute dispersion in Poiseuille flows of viscoelastic fluids for space applications provides valuable insights into the behavior of solute transport in these complex flows. The results will contribute for a better understanding of solute dispersion mechanisms in viscoelastic fluid flows and can aid in the design and optimization of processes and systems in space applications. Higher studies or future works in this area can give rise to these more empirical findings to explore more complex flow scenarios and investigate the impacts in the additional parameters on solute dispersion in viscoelastic fluid flows.

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