Viscoelastic modeling of the diffusion of polymeric pollutants injected into a pipe flow

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Abstract This study focuses on the transient analysis of nonlinear dispersion of a polymeric pollutant ejected by an external source into a laminar pipe flow of a Newtonian liquid under axi-symmetric conditions. The influence of density variation with pollutant concentration is approximated according to the Boussinesq approximation and the nonlinear governing equations of momentum, pollutant concentration are obtained together with an Oldroyd-B constitutive model for the polymer stress. The problem is solved numerically using a semi-implicit finite difference method. Solutions are presented in graphical form for various parameter values and given in terms of fluid velocity, pollutant concentration, polymer stress components, skin friction and wall mass transfer rate. The model can be a useful tool in understanding the dynamics of industrial pollution situations arising from improper discharge of hydrocarbon pollutants into, say, water bodies. The model can also be quite useful for available necessary early warning methods for detecting or predicting the scale of pollution and hence help mitigate related damage downstream by earlier instituting relevant decontamination measures.

Keywords Axi-symmetric flow · Polymeric pollutant dispersion · Oldroyd-B model Buoyancy forces · Semi-implicit finite difference method

1 Introduction

Spread of pollutants in a fluid flow depends largely on concentration coefficients [2]. These can be determined empirically for each type of pollutant. Investigations such as Ref. [3] and also the current one can help identify the pollutant physical properties (and the related mathematical parameters) likely to cause the greatest harm in spreading the pollutant downstream. The importance of these kind of investigations as well as the complimentary experimental works, say in, large scale water treatment and redistribution networks thus makes them of great relevance [4–9].

It should however be remarked that to date, the literature on the transient analysis of problem consisting of buoyancy effects and nonlinear pollutant injection is still quite sparse [10]. Moreover, investigations on polymeric pollutants is practically absent from the current literature and hence most pollution investigations have been carried out under Newtonian assumptions. Polymer blends often lead to products of superior quality [11], and hence there has been an ever increasing growth of the polymer industry. Most such products (from pharmaceuticals to beauty products) are liquid by nature and so are the waste products derived from their manufacture. Such waste products usually find their way into, say, water sources into which they are discharged...
by unscrupulous industries looking for rapid and cheap disposal channels of such waste.

The current investigation thus extends the Newtonian models in Ref. [10], to the viscoelastic regime. We thus suppose that a polymeric pollutant is introduced into a cylindrical pipe flow of a Newtonian liquid via an external source and proceed, under Boussinesq approximations, to investigate the transient diffusion and resultant spatial-temporal distribution of flow quantities.

In Sect. 2 the model problem is formulated and in particular the mathematical governing equations, initial and boundary conditions are outlined. In Sect. 3, the finite difference schemes that will be employed in the solution process are presented, followed by graphical results and discussions in Sect. 4.

2 Formulation of the problem

We consider a transient problem of fluid flow and nonlinear dispersion of a polymeric pollutant in a cylindrical pipe as shown in Fig. 1.

In order to derive the governing equations, the following assumptions are made:

(1) The pollutant-free fluid is viscous and incompressible.
(2) Initially, the flow is fully developed through a long cylindrical pipe. The flow is assumed to be axisymmetric and unidirectional in the axial (z) direction.
(3) At time $t > 0$, a polymeric pollutant is injected into the flow from an external source. As in Ref. [10], the pollutant is introduced into the flow via a distributed source around the pipe wall and is thus assumed to spread throughout the flow thereafter by radial diffusion. The uniform distribution of the source along the pipe (axial direction) and around the pipe (angular direction) means that the axial and angular diffusion as well as the convective motion of the pollutant would be negligible compared to the radial diffusion.
(4) It is thus idealized that the polymeric pollutant in thus injected uniformly throughout the wall with constant concentration $C_w$ and spreads throughout the pipe flow by radial diffusion. On diffusion into the pipe and mixing with the Newtonian solvent, the polymeric pollutant gradually forms a polymeric (viscoelastic) liquid within the pipe. The strength of the physical viscoelastic properties, say the polymer viscosity or the relaxation time, in turn lead to an internal pollutant source of strength $S(C)$, which depends on the prevailing concentration of pollutant $C$.
(5) The viscosity of the fluid as well as the pollutant mass diffusivity then vary with the concentration of the polymeric pollutant. In particular, solvent viscosity ($\mu_s$) decreases and polymer viscosity ($\mu_p$) increases with increasing pollutant concentration. The total viscosity ($\mu = \mu_s + \mu_p$) is also expected to increase with pollutant concentration.
(6) After the onset of pollutant injection, the fluid contains both solvent and polymeric components and is hence modeled using the Oldroyd-B constitutive equation.

(7) The influence of density variation with pollutant concentration is considered only in the body-force term of the momentum equation and is approximated according to the Boussinesq approximation.

![Fig. 1 Flow configuration and coordinate system](image)

The variables of interest are the velocity field $u = (u(r, t), 0, 0)$, polymer stress $\tau$ and pollutant concentration $C$. Under laminar flow conditions, the problem is reduced mathematically to a transient coupled fluid flow and mass transfer problem given in one dimension as

$$\frac{\partial u}{\partial t} = -\frac{\partial P}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \tau_{12} + \tau_{12} \frac{\partial u}{\partial r} \right) + \rho g \hat{z}(C - C_0),$$

$$\frac{\partial C}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r D_s \frac{\partial C}{\partial r} \right) + \frac{\partial}{\partial r} \left( \tau_{12} \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial r} \left( \frac{1}{r^2} \frac{\partial u}{\partial r} \right) + S(C),$$

where the upper convected derivative $\nabla_t^u$ and the deformation rate tensor $\dot{S}$ are defined respectively as

$$\nabla_t^u = \frac{D}{Dt} \nabla_t^u - \nabla_t^u \cdot \dot{u},$$

$$\dot{S} = \frac{1}{2} \left[ \nabla_t^u + (\nabla_t^u)^T \right].$$

Equation (2) for mass transfer under viscoelastic conditions, modeled by Eq. (3), are analogous to the equations for heat transfer in viscoelastic fluids, see for example Refs. [12–14] as well as the references cited therein. In particular, the four terms on the right hand side of Eq. (2) represent respectively the radial diffusion of pollutant, viscous decontamination, polymeric advection and pollutant internal source, the last of which is analogous, say to exothermic heat release.