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# NUMERICAL INVESTIGATIONS OF PASSIVE SCALAR TRANSPORT IN TURBULENT TAYLOR-COUETTE FLOWS: CODE VALIDATION 

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#### Abstract

The highly turbulent flow occurring inside (electro)chemical reactors requires accurate simulation of scalar mixing if CFD methods are to be used with confidence in design. This has motivated the present paper, which describes the implementation of a passive scalar transport equation into a hybrid spectral/finite-element code. For this purpose, direct numerical simulations (DNS) and Large Eddy Simulation (LES) have been performed to study the effects of the gravitational and the centrifugal potentials on the stability of incompressible Taylor-Couette flow. The flow is confined between two concentric cylinders and only the inner cylinder is allowed to rotate while the outer one is at rest. The Navier-Stokes equations and the uncoupled convection-diffusion-reaction (CDR) equation are solved using a code named SFELES which consists on spectral development in one direction combined with a finite element discretisation in the two remaining directions. The performance of the LES code is validated against published DNS data for a channel flow for the velocity and scalar statistics with good agreement between the current LES predictions and DNS data.


## INTRODUCTION

The fluid flow in the annulus between a rotating inner cylinder and fixed concentric outer cylinder has been extensively investigated for more than a century. The basic flow, known as Couette flow, continues to be a paradigm for experimental and theoretical studies of hydrodynamic stability and transition. The importance of TaylorCouette flow resides in the richness of flow regimes existing between laminar and turbulent flow, that is, several transition stages exist before the flow becomes turbulent.
Most research has been directed toward the stability of the flow with only minor attention to the supercritical velocity field that develops in the annulus. However, an understanding of the velocity field is crucial to engineering problems such as mixing and separation processes in the Couette device. Traditional approaches for studying the transition problems are flow visualization, spectral analysis, torque and heat/mass transfer.
The behavior of a Newtonian fluid confined to the annulus depicted in Fig. 1 (with a stationary outer cylinder and without axial flow) can be characterized by the azimuthal Reynolds number based on the gap between cylinders and angular velocity $\omega$, that is, $R e=\omega r_{i}\left(r_{o}-r_{i}\right) / v$ or by Taylor Number $\operatorname{Ta}=\operatorname{Re}\left(d / r_{i}\right)^{0.5}$, the ratio of the inner to outer cylinder diameters denoted by $\eta=r_{i} / r_{o}$, the aspect ratio $\Gamma=H / d$ and the imposed periodic
length in the transverse direction $\lambda_{z}$. The conventional length scale is the gap between cylinders $d=r_{o}-r_{i}$.

As $R e$ increases to a critical value, $R e_{c}$, the flow undergoes the first transition from laminar circular Couette flow (CCF) to laminar vortex flow (LVF) [1]. A number of velocity fiels measurements for laminar vortex flow have been made at single points. Only one component (the radial velocity $\left(u_{r}\right)$, the axial velocity $\left(u_{z}\right)$, or the azimuthal velocity $\left(u_{\theta}\right)$ was measured using laser Doppler velocimetry (LDV) [2, 3, 4]. All of these velocity measurements were used to validate the perturbation expansion theory developed by Davey [5]. Particle image velocimetry (PIV) was used to measure $u_{r}$ and $u_{z}$ in a meridional plane for laminar vortex flow by Wereley and Lueptow [6]. The measured velocity field matched Davey's theoretical field. As $R e$ is further increased above $R e_{c}$, the system exhibits a sequence of distinct time-independent and timedependent flow regimes before the onset of turbulence is reached. The first of these secondary instabilities occurs when LVF gives way to wavy vortex flow (WVF). WVF is characterized by travelling azimuthal waves superimposed on the inflow and outflow boundaries of the Taylor vortices. The flow field is unsteady and the vortices periodically expand and contract, compared to LVF, which is steady and axisymmetric. Upon a further increase in Re, WVF undergoes a transition to weakly turbulent wavy vortex flow, where turbulent eddies are superimposed on the wavy vortex structure. At higher Reynolds number $R_{e t}$, the azimuthal waves disappear and the flow is in the turbulent vortex flow (TVF) regime. The phenomena of the reemergence of azimuthal waves occur when Re is in a range slightly above $R e_{t}[7]$.

Coles [8] performed a flow visualization with suspended aluminum particles. His experiments detected azimuthally periodic waves which traveled around the inner cylinder superposed on the Taylor cells. Coles observed 26 different stable states for a fixed Reynolds number by varying the inner cylinder rotational speed slowly. Coles [8] also recorded approximately 75 transitions from one state to another by increasing the Reynolds number from 114 to 1348. These transitions were labeled by the number of Taylor vortex pairs and the number of azimuthal waves. Therefore, he was successful in showing that the final state was not unique and was dependent on both the Reynolds number and the flow history. He also concluded that, regardless of the state, the angular velocity of these waves was nearly 0.34 times the angular velocity of the inner cylinder. The wave speed, which was correct for his experimental setup, was found, later on, to be a function of radius ratio.

Numerical simulations for axisymmetric isothermal TaylorCouette flow have been performed by Meyer [9] using a finite difference technique. Computational work of steady axisymmetric Taylor vortex flow by a transient implicit method was also performed by Alziary De Roquefort et al. [10]. Numerical calculation of time dependent Taylor vortex flows in a finite-length annulus was done by Neitzel [11]. The transient development of a Taylor vortex structure was discussed and the axial wavelength was compared with experimental results for an impulsively started cylinder. Wave speeds of traveling waves have also been computed
numerically for axially periodic flows in infinite-length cylinders with a pseudospectral technique by King, et al. [12]. Their results showed that the wave speed, for a given radius ratio, decreases as Reynolds number increases until a plateau is reached. They also concluded that there was a much weaker dependence of the wave speed on the axial wavelength, azimuthal wave number as well as the aspect ratio.
The transition from Taylor vortex flow to wavy vortex flow was also numerically studied by Edwards et al. [13]. Their results of the critical Reynolds number for the onset of wavy vortex flow, azimuthal wave numbers and wave speeds were in good agreement with experimental values for a radius ratio $\eta=0.87$ and aspect ratios $\Gamma$ ranging from 8 to 34 . Similar computational investigations of Taylor vortex flow and wavy vortex flow were also conducted by Marcus [14, 15]. He used a fractional step scheme and solved the equations pseudospectrally. Marcus conjectured that the traveling waves were not shear instabilities associated with inflection points of the azimuthal flow but, instead, there were a secondary instability caused by the strong radial motion in the outflow boundaries of the Taylor vortices. He also demonstrated numerically that at the point of onset of the traveling waves, the speed of the waves was equal to the angular velocity of the fluid at the center of the Taylor vortices. Coughlin and Marcus [16] performed numerical simulations of modulated waves in Taylor-Couette flow using a three-dimensional initial value code for imposed values of the axial and azimuthal periodicity. They showed that periodic traveling waves become unstable to quasi-periodic modulated waves while increasing Reynolds numbers.

The effects of a radial temperature gradient on the stability of Taylor-Couette flows have been the subject of considerable investigation $[17,18]$. Stability analyses show that when gravity is neglected and the Reynolds number is sufficiently high the Taylor cells are stabilized when $T_{i}>T_{o}$ and destabilized when $T_{o}>T_{i}$ [19]. Roesner [20] included the effect of gravity through the Boussinesq approximation but only considered axisymmetric disturbances. He showed that isothermal Taylor cells are stabilized by both negative and positive radial heating and the stability boundaries are perfectly symmetric with respect to the direction of radial heating. Ali and Weidman [17] tested stability with respect to non-axisymmetric disturbances of both toroidal and helical type and found that the number of critical modes increased for large radius ratio.

An experimental study was performed by Kataoka, et al. [21] with the aid of an electrochemical technique under the assumption of analogy between heat and mass transfer. The author reported that the regular sinusoidal variation of the Sherwood number (Sh) is distorted by an added axial flow and both the mean and the amplitude are greatly reduced. Ball et al. [22] performed a parametric study of the mean heat transfer rates across the annular gap for three different radius ratios. Their results show that the heat transfer coefficient can be described by a power-law relationship and correlated as function of the Reynolds number and radius ratio.

Taylor vortex systems have been employed for a number of varied chemical and biochemical applications where they can be used as
reactors. The reactants can be fed into the top and bottom of the annulus at equal rates so that there is no axially imposed flow. Reactors operating in this way have been studied by Campero and Vigil [23], Tam and Swinney [24] and Vastano et al. [25]. This type of Taylor-vortex reactor approximates to a one-dimensional reaction-diffusion device.
In laminar Couette flow, no transport is assumed to occur in the radial or axial directions since motion is confined to the azimuthal direction only. Mass transport in concentric cylinder systems occurs by intra-vortex mixing and inter-vortex exchange. Intra-vortex mixing consists of a tangential (circumferential) dispersion with axial and radial mixing. In laminar Taylor vortex flow, the tangential dispersion is weak [26,27] and numerical models [28] indicate weak radial and axial mixing in the vortex core for Taylor flow. In contrast, layers of fluid near to vortex boundaries are readily mixed.
Ryrie [29] showed that with even for very small deviations from laminar Taylor vortex flow to wavy vortex flow, the fluid trajectories became chaotic, even in the absence of molecular diffusivity, resulting in an enhanced effective diffusivity or axial dispersion. From numerical simulations of the flow field (which agree with experimental observations), Rudolph et al. [30] showed that up to $50 \%$ of the volume of a vortex is transported in and out of a vortex in one azimuthal wave period. They verified Ryrie's findings in terms of chaotic particle paths and suggested that axial scalar transport is substantially increased over molecular diffusion. They proposed that optimum fluid transport between vortices takes place at Taylor Number $T a=253$ and that mixing and transfer decrease at both higher and lower Ta values than the required one for wavy vortex flow.


Figure 1. Sketch of the reactor with Taylor-Couette geometry.

In the last twenty years, Direct Numerical Simulations (DNS) have modified the way turbulent flows are studied. By providing new tools to investigate the instantaneous threedimensional structure of turbulent flows, DNS have allowed significant advances both in the understanding and the modeling of turbulence. However, DNS are restricted to low Reynolds numbers so that Large Eddy Simulations (LES) are preferred in practical applications. In order to further enhance the
confidence level in the results of the LES model, direct numerical simulations (DNS) of a turbulent pipe flow with a passive scalar has been performed for a Schmidt number of 0.7 and 5.
More detailed understanding has been gained and more complex models have been possible to explore and validate through the advent of direct numerical simulations (DNS). The first study of this kind was the DNS of channel flow with an imposed mean scalar gradient [31]. In the simulations of Kim and Moin [31] the Reynolds number, $R e_{\tau}$, based on the friction velocity, $u_{\tau}$, and the channel half width, $\delta$, is 180 and the Prandtl numbers used are $0.1,0.71$ and 2.
In the channel flow DNS of Kawamura et al. [32], a turbulent Reynolds number $R e_{\tau}=180$ and Prandtl numbers in the range $0.025-5$ are studied. In these studies the iso-flux boundary condition is applied and detailed budgets for the scalar variance, its dissipation rate and the scalar fluxes are presented.

## 1. MATHEMATICAL FORMULATION

### 1.1 LES methodology

A large eddy simulation contains only a range of the largest scales of a turbulent flow. The omitted small scales have an effect on the large scales because the problem is nonlinear. LES models are needed to account for this effect. The equations for an LES field are derived by applying a lowpass filter to the equations for the unfiltered field. New terms, often called sub-grid-scale (SGS) terms which are functions of the unfiltered field, appear. Models like the Smagorinski model replace such terms with others that depend on the LES field alone.

$$
\begin{align*}
\frac{\partial \tilde{u}_{i}}{\partial x_{i}} & =0  \tag{1}\\
\frac{\partial \tilde{u}_{j}}{\partial t}+\frac{\partial}{\partial x_{j}}\left(\tilde{u}_{i} \tilde{u}_{j}\right) & =-\frac{1}{\rho} \frac{\partial \widetilde{p}}{\partial x_{i}}+\frac{\partial^{2} \tilde{u}_{i}}{\partial x_{j} \partial x_{j}}-\frac{\partial \tilde{\tau}_{i j}^{S G S}}{\partial x_{j}} \tag{2}
\end{align*}
$$

where the symbol ( $\sim$ ) denotes an implicit operator
filtering and

$$
\tilde{\tau}_{i j}^{S G S}=\tilde{u}_{i} \tilde{u}_{j}-{\widetilde{u_{i}} \tilde{u}_{j}}
$$

This term which accounts for the effects of the unresolved scales, is called the subgrid-scale (SGS) Reynolds stress, and must be modeled via a SGS model.
These filtered Navier-Stokes equations govern the motion of the largest and energy-carrying scales of the flow, while the subgrid Reynolds stress term accounts for the effect of the unresolved small scales on the resolved ones. This term gives rise to a closure problem and must be modeled through a subgrid scale model. In practice, for a finite element discretization, the filtering operator ( . .) is implicit and linked to the resolution of the grid which is not able to capture turbulent scales smaller than a certain characteristic length $\Delta$. Most of the subgrid scale
models in use are commonly referred to as eddy viscosity models.

### 1.2 Smagorinski Model

The Smagorinski model [33] is certainly the most commonly used SGS model. A Boussinesq approximation is first made, in which the SGS Reynolds stress is assumed proportional to the resolved strain:

$$
\begin{equation*}
\tilde{\tau}_{i j}^{S G S}=2 \nu_{t} \tilde{S}_{i j}+\frac{1}{3} \tilde{\tau}_{l l} \delta_{i j} \tag{3}
\end{equation*}
$$

Where $\tilde{S}_{i j}=\frac{1}{2}\left(\frac{\partial \tilde{u}_{i}}{\partial x_{j}}+\frac{\partial \tilde{u}_{j}}{\partial x_{i}}\right)$ is the strain rate tensor of the filtered field, and $v_{t}$ is termed the eddy viscosity. The length scale is calculated from $l_{s}=C_{s g s} \Delta$, where $C_{s g s}$ is the Smagorinsky constant and the filter width $\Delta$ is obtained from $\Delta=\Delta_{r} \Delta_{z} \Delta_{\theta}$, with $\Delta_{r}, \Delta_{\theta}$ and $\Delta_{z}$ being the local cell size in the $r, \theta$ and $z$ directions respectively. For the sake of clarity, this implicit filtering operator symbol ( $\cdot$ ) is dropped hereafter. Several definitions have been proposed for this term. One of the most common definitions in use is the Smagorinski model where:

$$
\begin{equation*}
v_{t}=\left(C_{s g s} \Delta\right)^{2} \sqrt{2 S_{i j} S_{i j}} \tag{4}
\end{equation*}
$$

$C_{s g s}$ is a constant. Lilly [34] evaluated the value of the $C_{s g s}$ constant to 0.18 while Deardorff [35] found that this coefficient must be reduced to 0.1 in the presence of shear.
When a similar filtering operation is applied to the transport equation for a conserved scalar $\phi$, the following equation is obtained:

$$
\begin{array}{r}
\frac{\partial \phi}{\partial t}+\frac{\partial}{\partial x_{j}}\left(u_{i} \phi\right)=D \frac{\partial^{2} \phi}{\partial x_{j} \partial x_{i}}-\frac{\partial J_{i}}{\partial x_{j}} \\
J_{j}=u_{j} \phi-u_{j} \phi=D_{t} \frac{\partial \phi}{\partial x_{j}} \tag{6}
\end{array}
$$

Where $J_{j}$ is the sub-grid flux of the scalar.
The eddy diffusivity, $D_{t}=\frac{v_{t}}{P r_{t}}$ for the subgrid-scale scalar flux, is modeled using a constant turbulent Prandtl number $\mathrm{Pr}_{\mathrm{t}}=0.35$.
1.3 Wale Model (Wall-Adapting Local Eddyviscosity)
Close to the wall, the turbulent fluctuations cannot be bigger than the distance to the wall. The subgrid scale model has to damp the unresolved structures. Nicoud et al. [36] showed that in the region close to the wall, the eddy viscosity should scale like $v_{t} \approx O\left(y^{3}\right)$ where y corresponds to the distance closed to the wall. Van Driest [37] introduced a wall function which damps the structures close to the wall. This method does not
lead to an appropriate scaling for eddy viscosity ( $\mathrm{v}_{t} \approx O\left(y^{3}\right)$ ).
However, it requires the evaluation of the wall distance which can be problematic in complex geometries. To circumvent this problem, Nicoud et al. [36] built a formula for $v_{t}$ which uses the symmetric and antisymmetric part of the strain tensor and leads to the appropriate scaling close to the wall:

$$
\begin{gather*}
g_{i j}=\frac{\partial u_{i}}{\partial x_{k}} \frac{\partial u_{k}}{\partial x_{j}}  \tag{7}\\
S_{i j}=\frac{1}{2}\left[\frac{\partial u_{i}}{\partial x_{j}}+\frac{\partial u_{j}}{\partial x_{i}}\right]  \tag{8}\\
S_{i j}^{d}=\frac{1}{2}\left[g_{i j}+g_{j i}\right]-\frac{1}{3} \delta_{i j} g_{k k}  \tag{9}\\
v_{t}=\left(C_{w} \Delta\right)^{2} \frac{\left(S_{i j}^{d} S_{i j}^{d}\right)^{3 / 2}}{\left(S_{i j} S_{i j}\right)^{5 / 2}+\left(S_{i j}^{d} S_{i j}^{d}\right)^{5 / 4}} \tag{10}
\end{gather*}
$$

This formulation uses strain tensor properties observed close to the wall for different flows. The $C_{w}$ constant was calibrated for different flow simulations, according to Nicoud et al. [36] experience $0.55 \leq C_{w} \leq 0.6$.

### 1.4 Numerical procedure

In the absence of body forces, the mass and momentum conservation governing equations with constant density are:

$$
\begin{align*}
& \frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u} \cdot \nabla \boldsymbol{u}=\frac{-1}{\rho} \nabla p+v \nabla^{2} \boldsymbol{u}  \tag{11}\\
& \frac{\partial \phi}{\partial t}+\boldsymbol{u} \cdot \nabla \phi=D \nabla^{2} \phi+S(\phi) \tag{12}
\end{align*}
$$

and the continuity equation is:

$$
\begin{equation*}
\nabla . \boldsymbol{u}=0 \tag{13}
\end{equation*}
$$

where $\mathbf{u}$ is the velocity vector, $p$ is the pressure, $\rho$ is the fluid density, $\phi$ is the scalar (i.e., concentration, temperature), $\nu$ is the kinematic viscosity, $D$ is the molecular diffusivity of $\phi$ and $S(\phi)$ is the chemical source term.

We advance the governing equations (incompressible Navier-Stokes equations and the convection-diffusion equation) in time in a $2^{\text {nd }}$ order accurate manner, by setting the following continuity and momentum residuals to zero at each new time step $n+1$ :

$$
\begin{gather*}
R_{C}^{n+1}=\nabla \cdot\left(u^{n+1}\right)=0  \tag{14}\\
\boldsymbol{R}_{M}^{n+1}=\left(\boldsymbol{u}^{n+1}-\boldsymbol{u}^{n}\right) / \Delta t+\nabla p^{n+1 / 2}-\frac{1}{2 R e} \nabla^{2}\left(\boldsymbol{u}^{n+1}+\boldsymbol{u}^{n}\right)  \tag{15}\\
+3 / 2 \nabla \cdot\left(\boldsymbol{u}^{n} \boldsymbol{u}^{n}\right)-1 / 2 \nabla \cdot\left(\boldsymbol{u}^{n-1} \boldsymbol{u}^{n-1}\right)=0
\end{gather*}
$$

Herein, the pressure and viscous terms are treated in an implicit manner using the Crank-Nicolson scheme, whereas the convective terms are treated explicitly using the $2^{\text {nd }}$ order Adams-Bashforth method.

### 1.5 Spatial representation

Due to the periodic boundary conditions in the azimuthal and axial directions Fourier modes are appropriate for the expansion of the velocity field as a function of $\theta$. It is then natural to represent any flow unknown $q$ (where $q$ represents either the pressure or any component of the velocity vector $u$ and the passive scalar $\phi$ ) by means of a truncated Fourier series in, at least, one of these directions. In cross planes formed by the two remaining directions, we introduce a finite element representation on an unstructured triangular mesh (P1 elements).
We use a cylindrical coordinate system (z, r, $\theta$ ) and discretize in the azimuthal direction using a spectral expansion:

$$
\begin{equation*}
q^{n}(z, r, \theta)=\frac{1}{N_{\theta}} \sum_{k=-N_{\theta} / 2}^{N_{\theta} / 2} \sum_{j=1}^{N_{N o t}} Q_{k, j}^{n} N_{j}(z, r) e^{\text {le } \theta} \tag{16}
\end{equation*}
$$

Note that to ensure the real-value of the solution, the Fourier coefficients must obey the symmetry relation:

$$
\begin{equation*}
\mathrm{Q}_{\mathrm{k}}=\mathrm{Q}_{-\mathrm{k}}^{*} \tag{17}
\end{equation*}
$$

### 1.6 Pseudo-spectral time integration scheme

It can be shown that the above approach allows decoupling the 3D linear problem (Eq. 15) to be solved at each time step into a series of decoupled 2D linear problems, one for each Fourier mode. Coupling still occurs through the (nonlinear) convective terms, which are, however, treated explicitly and therefore do not complicate the (costly) linear solution phase. For the complete technical details of the discretization procedure outlined above, the reader is referred to [38, 39].

The discretized equations can be easily computed directly in terms of the Fourier components, except for the convective terms, which couple each Fourier mode to all others. The convective terms are therefore computed in physical space and then transformed to Fourier space using the Fast Fourier Transform (FFT) algorithm. The basic idea behind this pseudo-spectral solution procedure is as follows:
1-Evaluate the convective terms in physical space, using the previously calculated un and un-1;
2-transform these terms to Fourier space using the FFT algorithm;
3-set up the linear problems corresponding to each Fourier mode;

4-apply appropriate boundary conditions for each Fourier mode;
5-solve the linear systems to obtain the updated solution unknowns $Q_{k, j}^{n+1}$ in Fourier space;
6-apply the inverse Fourier transform to obtain the updated unknowns qn+1 in physical space.

For more details on the implementation and in particular the parallelization approach taken, the reader is referred to [38, 39].

## 2. CODE VALIDATION

### 2.1 Circular Couette flow

An in prior code validation has been conducted by simulating circular Couette flow. For $\eta=0.9$, the critical Reynolds number and Taylor number for the onset of Taylor vortices are 131.61 and 41.3 respectively [40]. A Reynolds number lower than this value gives rise to pure Couette flow. An analytical solution for Couette flow exists and shows a non-zero azimuthal velocity with a radial dependence (Eq. 18). The axial and the radial velocities are identically zero. As shown in figure 2 the numerical solution obtained for $\eta=0.875$, $\operatorname{Re}=50$ and $\lambda_{z}=2.5$ agrees well with the analytical solution for Couette flow ( $\mathrm{U}=1$ ).

$$
\begin{equation*}
\frac{u(r)}{U}=\frac{\eta}{1-\eta^{2}}\left(\frac{r_{o}}{r}-\frac{r}{r_{o}}\right) \tag{18}
\end{equation*}
$$



Figure 2. Analytical and numerical tangential velocity profile for circular Couette flow

### 2.2 Steady inhomogeneous CDR equation

The code for solving the governing equations is also tested and compared with known analytical solutions (steady inhomogeneous CDR equation)

$$
\begin{equation*}
\mathrm{u} \frac{\partial \phi}{\partial \mathrm{x}}-\mathrm{D} \frac{\partial^{2} \phi}{\partial \mathrm{x}^{2}}+\mathrm{c} \phi=\mathrm{S} \tag{19}
\end{equation*}
$$

c denotes the reaction coefficient.
To allow comparison with the analytic solution (figure 3), we consider a second test problem which involves constant coefficients: $u=1, D=-1, c=-2$ and $f=\cos x-3 \sin x$. Subject to Dirichlet-type boundary condition, the exact solution to the inhomogeneous convection-diffusion- reaction equation is derived as:


Figure 3. A comparison of exact and numerical solutions for the one-dimensional steady inhomogeneous CDR equation.

We also carried out computations on continuously refined grids, namely, h/20; h/40; h/60; h/80; h/100; h/160, and cast prediction errors in their L2-norms. As figure 4 shows, the rate of convergence obtained using the proposed code is as 1.827 .


Figure 4. The rate of convergence plot for the developed code

## 3. RESULTS

### 3.1Transient development of Taylor vortices

If Taylor number exceeds the critical number of 41.3, the disturbances or the vortices from the ends propagate to the central region due to Taylor instability [8]. The transient development of axisymmetric Taylor vortex flow for $T a=56$ was studied by the code. The later was run on in an annulus With a height to gap aspect ratio equal to 6.25 with a uniform grid $32(\mathrm{r}) \times 64(z) \times 32(\theta)$ and a time step 0.0002 . Fig. 5(a), (b), (c) and (d) plot the streamlines for selected solutions at different time steps. At first, the flow is quickly developed to circular Couette flow from rest, and a initial vortex cell is developed from each of the two ends due to the end effect (Fig. 5(a)). After the cells grow to the full size and intensity, they propagate toward the central region and form the second pair of cells (Fig. 5(b)). After they gain size and intensity, the third pair of the cells begins to form (Fig. 5(c)). Eventually, the entire gap is filled with cells of equal size and intensity (Fig. 5(d)).


Figure 5. Streamlines at different time steps: (a) cells start to form from the ends; (b) second groups of cells starts to form; (c) the inner cells start to form; (d) close to fully developed cells.

At high Rayleigh numbers, the flow becomes timedependent and complex with numerous states and transitions as observed by Coles [8]. Also, the code was tested at Taylor vortex regime with $T a=90$. This low value of the Taylor number, for which the flow is still steady and axisymmetric, is used to assess the performance of the code. The following integral flow quantities
$E=\frac{1}{2 H d^{2}\left(\omega r_{i}\right)^{2}} \int_{0}^{2 \pi} \int_{0}^{H} \int_{r_{i}}^{r_{o}}|\boldsymbol{u}|^{2} r d r d z d \theta$
$L=\frac{1}{2 H d^{3} \omega r_{i}} \int_{0}^{2 \pi} \int_{0}^{H} \int_{r_{i}}^{r_{0}} u_{\theta} r^{2} d r d z d \theta$
$\varepsilon=\frac{1}{2 H\left(\omega r_{i}\right)^{2}} \int_{0}^{2 \pi} \int_{0}^{H} \int_{r_{i}}^{r_{0}}|\nabla \times \mathrm{u}|^{2} r d r d z d \theta$
are compared, with good agreement (table 1), to literature results [15,41] and Manna and Vacca [41].

Table 1
Integral quantities for Taylor-Couette flows at $T a=90$

|  | Present <br> work | Marcus <br> $[1984 \mathrm{a}]$ | Manna and <br> Vacca [1999] |
| :--- | :--- | :--- | :--- |
| Kinetic E | 6.17 | 6.13 | 6.13 |
| Momentum L | 142 | 142 | 142 |
| Enstrophy $\mathcal{E}$ | 41.2 | 41.0 | 41.1 |

### 3.2 Heat transfer

A fixed geometry is considered in the present study, with $\Gamma=10$ and $\eta=0.5$. The annular gap between the two cylinders is filled with a Boussinesq fluid with Prandtl number $\operatorname{Pr}=0.71$.

The inner cylinder of the annulus is rotating at a constant speed, while the outer cylinder is stationary. A temperature difference is imposed between the isothermal inner and outer cylinders, with the inner cylinder being hotter $\left(T_{i}>T_{o}\right)$. Both ends are taken to be adiabatic and stationary.

The rotational speed of the inner cylinder, characterized by $T a$, is gradually increased from zero without thermal buoyancy effects. A series of steady state results for different values of $T a$ (up to $T a=27.3$ ) is shown in figure 6 . Within the range $0<T a<$ 25.35, the system reaches the steady state condition quickly. At $T a=$ 11.7, two vortices appear immediately adjacent to both end walls (Figure 6a) due to Ekman pumping [42]. The vortices circulate in the sense that the fluid is moving inward (towards the inner cylinder) along the two end walls. By increasing Ta from $T a=11.7$ to $T a=19.5$, the two vortices at the ends become stronger and induce two more vortices towards the center (figure 6b). The induction of the vortices continues with further increases in Ta from $T a=19.5$ up to $T a=25.35$ (figure $6 \mathrm{c}-\mathrm{d}$ ). This phenomenon has previously been reported [10, 42].


Figure 6. Streamlines for isothermal Taylor-Couette flow
(a) $\mathrm{Ta}=11.7$, (b) $\mathrm{Ta}=19.5$, (c) $\mathrm{Ta}=23.4$, (d) $\mathrm{Ta}=25.35$ and (e) $\mathrm{Ta}=27.3$.

Unlike the quick transient response encountered for the lower Ta results described above, it is noticed that the system adjusts itself gradually and takes much longer to reach steady state when $T a$ is increased from $T a=25.35$ to $T a=27.3$. Vortices of comparable sizes begin to fill the domain (figure 6e). By comparing the results for $T a=25.35$ and $T a=27.3$, the spontaneous onset of the vortices in the center region of the domain and the strength of these vortices indicate that these central vortices are not just the result of the end wall effect (Ekman layers).
Based on the linear stability analysis, the critical Taylor number for an infinite annulus with a radius ratio of $\eta=0.5$ is $T a_{c}=$ 26.6. Below $T a_{c}$, a pure shear flow (circular Couette flow) caused by the rotating cylinders exists, while above $T a_{c}$, the onset of the Taylor vortices is predicted. However, in the current numerical study, vortices occur below and above $T a_{c}$ in a finite annulus. The mechanism triggering the vortices below $T a_{c}$ in a finite annulus is the end wall effect, which is absent in an annulus of
infinite length. On the other hand, the mechanism triggering the vortices above $T a_{c}$ is the hydrodynamic instability of the system, which is present regardless of the end walls. Therefore, when the Taylor number is increased from $T a=25.35$ (below $T a_{c}$ ) to $T a=$ 27.3 (above $T a_{c}$ ), due to the change in the stability of the flow, a significant change in the flow field is detected.

### 3.3 Mass transfer

For the concentration problem, the boundary conditions are:

$$
\begin{array}{ll}
\phi=0 & \forall z, r=r_{i} \\
\phi=1 & \forall z, r=r_{o}
\end{array}
$$

First, a study was performed for the ferri-ferrocyanide solution containing the supporting electrolyte 100 mM NaOH with a pH of approximately of 13 . The properties of this solution are: the diffusion coefficient is $D=5.6 \times 10^{-10} \mathrm{~m}^{2} / \mathrm{s}$, a valency number $n=1$, a nominal concentration $\phi_{0}$, a kinematic viscosity $v=10^{-6} \mathrm{~m}^{2} / \mathrm{s}$ (yielding a large Schmidt number $\mathrm{Sc}=1785$ ). The following electrochemical reaction is considered at CDR which is the inner (rotating) cylinder:

$$
\mathrm{Fe}(\mathrm{CN})_{6}^{3-}+e^{-} \rightarrow \mathrm{Fe}(\mathrm{CN})_{6}^{4-}
$$

An analytical solution for the diffusion-convection problem at $R e>1$ does not exist. Our simulations yield good agreement with the empirical relationship of Eisenberg [43] which gives the limiting current density $j$ as a function of the rotation speed:

$$
\begin{equation*}
j=0.0791 n F \phi_{0} U_{\text {rot }}\left(\frac{2 r U_{\text {roti }}}{v}\right)^{-0.3}\left(\frac{v}{D}\right)^{-0.644} \tag{24}
\end{equation*}
$$

where F is Faraday's constant, $U_{\text {rot }}$ is the tangential velocity at the rotating electrode. Equation (24) is valid in a wide interval of Reynolds numbers. In our simulations the limiting current density was calculated as:

$$
\begin{equation*}
j=-n F D \nabla \phi \tag{25}
\end{equation*}
$$

where $\nabla \phi$ is the gradient of concentration averaged in time near the surface of the electrode. The numerical solution has a better agreement with [43] at small rotation speeds (figure 7) mainly solutions obtained with LES-Wale formulation.


Figure 7. Comparison of the numerical data with the empirical Eisenberg's relation Eq. (24) at the Reynolds numbers $\operatorname{Re}<10000$. The dimensions of the reactor are: $r i=6 \mathrm{~mm}$,

$$
r_{o}=35 \mathrm{~mm}, H=50 \mathrm{~mm} .
$$

The Sherwood number at the outer cylinder was compared to experiments [21] with very good agreement (figure 8). Variation from experiment was due to a high Schmidt number of the experiments $(S c=3000)$. Note that the $\mathrm{Sc}=5.0$ case showed better agreement with the experiments than one of $\mathrm{Sc}=0.71$. The Reynolds number for the CDR simulation was chosen according to previous experimental work [21].


Figure 8. Sherwood number at the outer cylinder. $\mathrm{Re}=3200$

### 3.4 Second order statistics

Computer resources limit LES and DNS to simple configurations and low Reynolds and Schmidt numbers (e.g. for pipe flow $\mathrm{Re}=5000$ and $\mathrm{Sc}=5$ ). For liquids, the Schmidt number is ranging from 100 to 1000 . Although both LES and DNS cannot achieve this, the present work can still contribute by examining the trends that occur when increasing Schmidt number (e.g. $\mathrm{Sc}=0.7$ versus $\mathrm{Sc}=5.0$ ).

Table2: Pipe flow - computational conditions

| Reynolds number | $2400\left(R e_{\tau} \approx 180\right)$ |
| :--- | :--- |
| Schmidt number | 0.7 and 5 |
| Grid number | $256 \times 128 \times 64$ |
| Grid spacing $\Delta r^{+}=0.14,2.44, \Delta z^{+}=4.44$, <br> (wall units) $r_{i} \Delta \theta^{+}=5.54$ |  |

Table 3: Taylor Couette flow - computational conditions

| Reynolds number | $3000\left(R e_{\tau} \approx 180\right)$ |
| :--- | :--- |
| Schmidt number | 0.7 and 5 |
| Grid number | $256 \times 128 \times 64$ |
| Grid spacing <br> (wall units) | $\Delta r^{+}=0.32,267, \quad \Delta z^{+}=3.44$, <br> $r_{i} \Delta \theta^{+}=5.54$ |

In order to assess the performance of the code, comparison of the rms of the velocities obtained from LES-Wale model with those from DNS and reference data from [44, 32] was first conducted as depicted in figure 9 .

Fluctuating velocity shows very good agreement with both DNS data from SFELES and [44, 32].


Figure 9. Pipe flow - Comparison of velocity rms values
The scalar fluctuations (figure 10) also display very good agreement with [32] near the wall. However, for regions away from the wall for $y^{+} \geq 15$ the present results tend to overpredict Kawamura's results.


Figure 10. Pipe flow - Comparison of scalar rms values
For Taylor-Couette flows, the fluctuating velocities show a remarkable similarity to those of channel flow (figure 11). This indicates that the turbulent velocity fluctuations might be similar in both configurations. However, the magnitude of the peak fluctuations is much less than the channel flows.
It should be observed that the shapes and the trends in the concentration fluctuations (figure 12) show that as Sc increases, the peak in the concentration fluctuations gets more pronounced and moves closer to the wall. The same trends were reported by [32] for a channel at $\mathrm{Re}=180$ and uniform heating from both walls from $\mathrm{Sc}=0.025$ to $\mathrm{Sc}=5$.


Figure 11. Taylor-Couette flow - Fluctuating velocity and scalar for $\mathrm{Sc}=0.7$ and $\mathrm{Sc}=5.0$


Figure 12. Taylor-Couette flow - rms values of scalar for different Schmidt numbers.

## CONCLUSION

In the present paper we have demonstrated the performance of implementation, including assessment testing, of a passive scalar equation in a code combining Spectral and Finite Elements discretisations of NavierStokes equations.

The numerical study here is all based on a case of rotating inner cylinder and resting outer cylinder with a sudden start from the rest. It is considered exploratory to demonstrate the code's ability to solve three-dimensional flow in axisymmetric geometries including passive scalar transport with uniform boundary and initial conditions with both LES and DNS methods

The resulting fluctuating velocity and scalar fields reproduce well the statistics (up to second-order). Good agreement was found between the results obtained from our code with literature.

## NOMENCLATURE

| QUANTITY | SYMBOL |
| :--- | :--- |
| Absolute temperature of inner <br> cylinder | $T_{i}$ |
| Absolute temperature of outer <br> cylinder | $T_{o}$ |
| Angular velocity | $\omega$ |
| Aspect ratio | $\Gamma=H / d$ |
| Boundary layer thickness | $\delta(x)$ |
| Critical Reynolds Number | $R_{e c}$ |
| Cylindrical coordinates | $r_{r} \theta, z$ |
| Distance from the wall | $y^{+}$ |
| Friction velocity | $u_{\tau}$ |
| Friction velocity Reynolds number | $R e_{\tau}$ |
| Gap between cylinders | $d=r_{o}-r_{i}$ |
| Hydraulic diameter | $d_{h}=2\left(\mathrm{r}_{\mathrm{o}}-\mathrm{r}_{\mathrm{i}}\right)$ |
| Inner diameter | $d_{i}$ |
| Inner radius | $\mathrm{r}_{\mathrm{i}}$ |
| Outer diameter | $d_{o}$ |
| Outer radius | $\phi$ |
| Passive scalar | $\mathrm{r}_{\mathrm{o}}$ |
| Periodic length in the transverse <br> direction | $\lambda_{z}$ |
| Ratio of the inner to outer cylinder <br> radii | $\eta=r_{i} / r_{o}$ |
| Reynolds Number | $R e=\omega r_{i}\left(r_{o}-r_{i}\right.$ |
| Taylor Number | $T a=R e\left(d / r_{i}\right.$ |
| Turbulent Prandtl Number | $R_{e t}$ |
| Turbulent Reynolds Number | $u$ |
| Velocity components in Cylindrical <br> coordinates $r, \theta, z$ <br> $u_{r}, u_{\theta}, u_{z}$ |  |

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