Abstract

BECKER, SID MARTIN. NUMERICAL MODELING OF A FALLING BIOCONVECTION PLUME IN A POROUS MEDIUM. (Under the direction of A.V. Kuznetsov.)

This thesis considers the bioconvective plume in a fluid saturated porous medium.

Bioconvective plumes arise as a result of an unstable distribution of micro-organisms. This unstable distribution occurs when the micro-organisms, heavier than, accumulate in the upper regions of the fluid. The plume transports cells and oxygen from the upper regions to the lower regions. This thesis attempts to find a steady state solution of the plume in a porous medium by an of implicit finite difference method. The parabolized governing equations are discretized in a series of implicit finite difference equations, and the resulting steady state solutions are presented. A similarity solution of the plume is also obtained for comparison purposes.

**NUMERICAL MODELING OF A FALLING BIOCONVECTION PLUME IN A
POROUS MEDIUM**

by
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Dedication

This thesis is dedicated to Dr. Jon Rust.

Biography

Sid Becker was born in Darmstadt, Germany on May 1, 1972.

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He likes it there.

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Introduction

Bioconvection is a phenomenon resulting from a density instability that arises when up swimming microbiological organisms that are denser than their surrounding fluid gather at regions near the upper surface. The accumulation of these organisms causes the upper layer to be denser than the region below and instability is introduced, which in turn leads to the development of bioconvective plumes [1-5].

Here we consider the microorganisms to be the oxytactic bacteria *bacillus subtilis*, as in Metcalfe and Pedley [6] and Hillebrandson, et al.[7]. These bacteria are oxygen consumers and thus they tend to swim from lower to higher oxygen concentrations. Oxygen diffuses from the free surface into the regions below, therefore, the bacteria tend to migrate to regions just below the free surface where the oxygen concentration is the highest. Because the bacteria are denser than the fluid, their accumulation near the surface causes the upper layer to become heavier than the lower layers. This instability causes the formation of bioconvective plumes. As these plumes begin to form, cells are drawn from the cell-rich upper fluid layer. Although the cell rich upper layer would eventually be depleted of cells, plume formation and development occurs in a much shorter time so the falling plumes may be assumed to be steady or at least quasi-steady. The plumes are also assumed to be axisymmetric. A schematic of a bioconvection plume is provided in Fig. 1.

Fig. 1 Schematic diagram of the bioconvection plume

As the cells are transported away from the surface, they continue to consume oxygen, and try to migrate towards higher oxygen concentrations. Although at regions far below the surface oxygen consumption by the cells depletes the fluid of oxygen to such an extent that the cells become inactive, this thesis focuses on the regions where all the bacteria are still active.

Metcalfe and Pedley [6] describes the falling plumes using a similarity solution. Kuznetsov, et al. [8] expand on Metcalfe and Pedley's work by finding a similarity solution of the plumes in a porous medium.

When it is considered helpful to dampen the convective effects brought on by bioconvection, a porous media (such as gauze) may be introduced as shown in Kessler [9]. Such a media should be sufficiently porous to allow the swimming and falling cells to penetrate through it. In this thesis the governing equations are discretized by using a conservative finite-difference scheme. A fully implicit scheme is used to obtain the steady state solutions of cell and oxygen concentrations and of the axial velocity profile. An iterative line-by-line tridiagonal matrix algorithm is used to solve the nonlinear discretized equations. A similarity solution is also obtained, the results of which are compared to the difference solution.

Governing Equations

The falling plume is described using a cylindrical coordinate system and is assumed to be axisymmetric. The governing equations are written using the Boussinesq approximation which, in this case, sets fluid properties to that of water except in the buoyancy term which is contained in the momentum equation. Darcy's law is used in the momentum equation to handle the effects of porosity.

Conservation of cells

The steady state equation for cell conservation is:

$$0 = \nabla \cdot (n\mathbf{U} + n\mathbf{V} - D_n \nabla n) \quad (1)$$

in which $\mathbf{U}$ is the bulk fluid filtration velocity, $D_n \nabla n$ describes the diffusion of cells, n is the concentration of cells $\left(\frac{\# \text{ cells}}{m^3} \right)$.

The term $\mathbf{V}$ describes the cell swimming along the oxygen gradient and is represented as:

$$\mathbf{V} = bW_c \nabla C \quad (2)$$

where bW_c is a constant that refers to the cells swimming along the oxygen gradient, and C is the dimensionless oxygen concentration and is defined as:

$$C = \frac{\tilde{C} - \tilde{C}_{min}}{\tilde{C}_0 - \tilde{C}_{min}} \quad (3)$$

The term $\tilde{C}_0$ is the concentration of oxygen at the free surface and $\tilde{C}_{min}$ is the minimum oxygen concentration required for the bacteria to remain active. This model assumes that the cells always have enough oxygen to remain active, i.e. $C > 0$.

Rearranging Eq. (1) and substituting Eq. (2) yields:

$$\nabla \cdot (n\mathbf{U} + nbW_c \nabla C) = \nabla (D_n \nabla n) \quad (4)$$

or

$$\nabla \cdot (n\mathbf{U}) + bW_c (\nabla \cdot (n \nabla C)) = D_n \nabla^2 n \quad (5)$$

In terms of cylindrical coordinate system, Eq. (5) is expressed as:

$$\begin{aligned} & v \frac{\partial n}{\partial z} + u \frac{\partial n}{\partial r} + bW_c \left(\frac{\partial n}{\partial z} \frac{\partial C}{\partial z} + \frac{\partial n}{\partial r} \frac{\partial C}{\partial r} + n \left(\frac{\partial^2 C}{\partial z^2} + \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) \right) \\ & = D_n \left(\frac{\partial^2 n}{\partial z^2} + \frac{\partial^2 n}{\partial r^2} + \frac{1}{r} \frac{\partial n}{\partial r} \right) \end{aligned} \quad (6)$$

where r is the radial coordinate, z is the axial coordinate, u is the radial velocity, and v is the axial velocity.

In the upper regions of the plume (where all the cells are active), the cell conservation

equation may be parabolized by neglecting the terms $\frac{\partial^2 n}{\partial z^2}$, $\frac{\partial n}{\partial z} \frac{\partial C}{\partial z}$, and $\frac{\partial^2 C}{\partial z^2}$.

Neglecting these terms and rearranging yields the parabolized conservation of cells equation:

$$v \frac{\partial n}{\partial z} + \left(u + bW_c \frac{\partial C}{\partial r} \right) \frac{\partial n}{\partial r} + bW_c n \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) = D_n \left(\frac{\partial^2 n}{\partial r^2} + \frac{1}{r} \frac{\partial n}{\partial r} \right) \quad (7)$$

Conservation of oxygen

The steady equation describing the conservation of oxygen is:

$$0 = -\nabla \cdot (C\mathbf{U} - D_c \nabla C) - \gamma_0 n \quad (8)$$

where D_c is the diffusivity of oxygen and $-\gamma_0 n$ describes the consumption of oxygen by the cells, and γ_0 is a constant characterizing the oxygen consumption rate.

Rearranging Eq. (8)

$$\nabla \cdot (CU) = D_c \nabla^2 C - \gamma_0 n \quad (9)$$

and describing in terms of the cylindrical coordinate system yields:

$$v \frac{\partial C}{\partial z} + u \frac{\partial C}{\partial r} = D_c \left(\frac{\partial^2 C}{\partial z^2} + \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) - \frac{\gamma_0 n}{\Delta C} \quad (10)$$

Equation (10) is parabolized by neglecting the term $\frac{\partial^2 C}{\partial z^2}$, which results in:

$$v \frac{\partial C}{\partial z} + u \frac{\partial C}{\partial r} = D_c \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) - \frac{\gamma_0 n}{\Delta C} \quad (11)$$

where $\Delta C = \tilde{C}_0 - \tilde{C}_{min}$.

Momentum equation

In Henri Darcy [10] a generalized relationship between flow rate in a porous medium and

applied pressure difference is defined as: $\nabla P = -\frac{\mu}{K} \mathbf{V}$. Using Darcy's law for a uniform

porous medium in conjunction with the steady Navier Stokes momentum equation yields:

$$(\mathbf{V} \cdot \nabla) \mathbf{V} = -\nabla P - \frac{\mu}{K} \mathbf{V} + \mathbf{F}_b \quad (12)$$

in which P is the total pressure, $\mathbf{F}_b$ is the body force, μ is the fluid dynamic viscosity (assumed to be that of water), and K is the permeability of the porous medium.

In a non-porous scenario, a moving fluid keeps its momentum in the absence of applied forces. However, this is not the case in a porous medium because the solid matrix that makes up the medium impedes the motion causing a change in momentum. Therefore the convective term $(\mathbf{V} \cdot \nabla) \mathbf{V}$ is removed from Eq. (12) and the resulting momentum equation is written:

$$0 = -\nabla P - \frac{\mu}{K} \mathbf{V} + \mathbf{F}_b \quad (13)$$

z-momentum equation

The axial component of Eq. (13) in cylindrical coordinates is

$$\frac{\partial P}{\partial z} + \frac{\mu}{K} v - \rho g = 0 \quad (14)$$

where ρ is the local fluid density, and g is gravity.

Noting that the total pressure, P , is composed of hydrostatic pressure, p_s , and pressure above hydrostatic, p .

$$P = p + p_s \quad (15)$$

using this definition of total pressure, Eq. (14) may be written as

$$\frac{\partial p}{\partial z} + \frac{\partial p_s}{\partial z} + \frac{\mu}{K} v - \rho g = 0 \quad (16)$$

The hydrostatic pressure gradient, $\frac{\partial p_s}{\partial z}$, is dictated by the fluid density outside the plume which is the density of water, ρ_w , so that:

$$\frac{\partial p_s}{\partial z} = \rho_w g \quad (17)$$

Substituting for the hydrostatic pressure gradient into Eq. (16) yields

$$\frac{\partial p}{\partial z} + \frac{\mu}{K} v - (\rho - \rho_w)g = 0 \quad (18)$$

The local density, ρ , is a combination of the cell density, ρ_n , and the water density, ρ_w , and it may be described as:

$$\rho = \rho_n x(\text{volume fraction of cells}) + \rho_w x(\text{volume fraction of water}) \quad (19)$$

or

$$\rho = \rho_n x(\text{volume fraction of cells}) + \rho_w x(1 - \text{volume fraction of cells}) \quad (20)$$

Defining the volume fraction of cells as $\frac{\left(\text{volume occupied by cells in } 1\text{m}^3 \right)}{\left(1\text{m}^3 \right)}$ and recalling

that the cell concentration is $n = \left(\frac{\# \text{ cells}}{m^3} \right)$ and introducing cell volume as $\theta = \left(\frac{m^3}{\text{cell}} \right)$, Eq.

(20) may be written as:

$$\rho = \rho_n n\theta + \rho_w x(1 - n\theta) \quad (21)$$

or

$$\rho - \rho_w = n\theta(\rho_n - \rho_w) \quad (22)$$

Defining $\Delta\rho$ is the difference between cell density and the water density and substituting Eq. (22) into Eq. (18), the axial - momentum equation may be written as:

$$\frac{\partial p}{\partial z} + \frac{\mu}{K} v - n\theta \Delta\rho g = 0 \quad (23)$$

r-momentum equation

The radial component of the momentum equation (13) is represented as:

$$\frac{\partial p}{\partial r} + \frac{\mu}{K} u = 0 \quad (24)$$

combined momentum equation

In order to reduce unnecessary computations, the excess pressure term, p , is removed from the from the r and z momentum equations as follows.

The axial z momentum equation (23) is differentiated with respect to radial coordinate, r ,

$$\frac{\partial^2}{\partial r \partial z}(p) + \frac{\partial}{\partial r} \left(\frac{\mu}{K} v \right) - \theta \Delta \rho g \frac{\partial}{\partial r}(n) = 0 \quad (25)$$

The radial r momentum equation (24) is differentiated with respect to axial coordinate, z ,

$$\frac{\partial^2}{\partial r \partial z}(p) + \frac{\mu}{K} \frac{\partial}{\partial z}(u) = 0 \quad (26)$$

Then Eq. (26) is subtracted from Eq. (25) yielding the combined momentum equation:

$$\frac{\mu}{K} \left(\frac{\partial v}{\partial r} - \frac{\partial u}{\partial z} \right) - \frac{\partial n}{\partial r} \theta \Delta \rho g = 0 \quad (27)$$

In parabolic approach $\frac{\partial u}{\partial z}$ may be assumed very small; neglecting this term in Eq. (27) yields

the parabolized combined momentum equation:

$$\frac{\mu}{K} \left(\frac{\partial v}{\partial r} \right) - \frac{\partial n}{\partial r} \theta \Delta \rho g = 0 \quad (28)$$

Continuity equation

The continuity equation using the Boussinesq approximation is

$$\nabla \cdot \mathbf{V} = 0 \quad (29)$$

In cylindrical coordinates Eq. (29) is written as:

$$\frac{1}{r} \frac{\partial(ru)}{\partial r} + \frac{\partial v}{\partial z} = 0, \quad (30)$$

Equations (1), (3), (6), and (7) or (8) must be solved subject to the following boundary conditions. Utilizing symmetry about $r=0$, the following boundary conditions are imposed at $r=0$:

$$\frac{\partial n}{\partial r} = 0, \quad \frac{\partial C}{\partial r} = 0, \quad u = 0, \quad \frac{\partial v}{\partial r} = 0 \quad (31)$$

At $r \rightarrow \infty$ the following boundary conditions are imposed:

$$n \rightarrow 0, \quad \frac{\partial C}{\partial r} \rightarrow 0, \quad v \rightarrow 0 \quad (32)$$

Integral Condition

An integral condition is used to check the accuracy of the computations. The integral condition is formulated using the conservation of cells equation (7) and the continuity equation (30).

The cell conservation equation (7) is multiplied by r and rearranged yielding:

$$rv \frac{\partial n}{\partial z} + r \left(u + bW_c \frac{\partial C}{\partial r} \right) \frac{\partial n}{\partial r} + rbW_c n \left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right) - rD_n \left(\frac{\partial^2 n}{\partial r^2} + \frac{1}{r} \frac{\partial n}{\partial r} \right) = 0 \quad (33)$$

or

$$ru \frac{\partial n}{\partial r} + \left[rbW_c \frac{\partial C}{\partial r} \frac{\partial n}{\partial r} + rbW_c n \frac{\partial^2 C}{\partial r^2} + bW_c n \frac{\partial C}{\partial r} \right] - \left[rD_n \frac{\partial^2 n}{\partial r^2} + D_n \frac{\partial n}{\partial r} \right] + rv \frac{\partial n}{\partial z} = 0 \quad (33b)$$

The continuity equation (30) is multiplied by $n r$ resulting in:

$$n \frac{\partial(ru)}{\partial r} + nr \frac{\partial v}{\partial z} = 0 \quad (34)$$

or

$$nu + nr \frac{\partial u}{\partial r} + nr \frac{\partial v}{\partial z} = 0 \quad (34b)$$

Equations (33b) and (34b) are added to each other resulting in:

$$\left[ru \frac{\partial n}{\partial r} + nu + nr \frac{\partial u}{\partial r} \right] + \left[rbW_c \frac{\partial C}{\partial r} \frac{\partial n}{\partial r} + rbW_c n \frac{\partial^2 C}{\partial r^2} + bW_c n \frac{\partial C}{\partial r} \right] - \left[rD_n \frac{\partial^2 n}{\partial r^2} + D_n \frac{\partial n}{\partial r} \right] + \left[rv \frac{\partial n}{\partial z} + nr \frac{\partial v}{\partial z} \right] = 0 \quad (35)$$

Equation (35) may be rewritten as:

$$\frac{\partial}{\partial r} \left[run + rbW_c n \frac{\partial C}{\partial r} - rD_n \frac{\partial n}{\partial r} \right] + \frac{\partial}{\partial z} [rvn] = 0 \quad (35b)$$

Equation (35b) is integrated with respect to r :

$$\int_0^\infty \frac{\partial}{\partial r} \left[run + rbW_c n \frac{\partial C}{\partial r} - rD_n \frac{\partial n}{\partial r} \right] dr + \int_0^\infty \frac{\partial}{\partial z} [rvn] dr = 0 \quad (36)$$

and by Leibnitz:

$$\int_0^\infty \frac{\partial}{\partial r} \left[run + rbW_c n \frac{\partial C}{\partial r} - rD_n \frac{\partial n}{\partial r} \right] dr + \frac{\partial}{\partial z} \int_0^\infty [rvn] dr = 0 \quad (36b)$$

yields:

$$run \Big|_0^\infty + rbW_c n \frac{\partial C}{\partial r} \Big|_0^\infty - rD_n \frac{\partial n}{\partial r} \Big|_0^\infty + \frac{\partial}{\partial z} \int_0^\infty [rvn] dr = 0 \quad (37)$$

Using the boundary conditions (31) and (32), Eq. (37) reduces to:

$$\frac{\partial}{\partial z} \int_0^\infty [rvn] dr = 0 \quad (38)$$

which means that $\int_0^\infty rvn dr$ does not change with depth, z .

If Q is defined as the cell flux entering the plume from the cell rich upper layer, then:

$$Q = 2\pi \int_0^{\infty} r v n dr = \text{constant} \quad (39)$$

Recalling Fig.1, inlet conditions are prescribed such that:

Axial velocity is zero outside the plume:

$$\begin{aligned} z = 0, r \leq R_0 : \quad v &= v_0 \\ z = 0, r > R_0 : \quad v &= 0 \end{aligned} \quad (40)$$

The radial velocity at $z = 0$ is zero:

$$z=0: \quad u_0 = 0 \quad (41)$$

It is also necessary to prescribe value of cell concentration at the inlet:

$$z=0: \quad n = n_0 \quad (42)$$

The terms R_0 , n_0 , and v_0 represent inlet values of plume radius, cell concentration and axial velocity respectively.

Imposing conditions (40), (41), and (42) on the integral described in Eq. (39), it follows that for the circular inlet cross-section of radius R_0

$$Q = \pi R_0^2 n_0 v_0 \quad (43)$$

Dimensionless Equations

Dimensionless governing equations

In order to greatly simplify the computation of the plume solution, the governing equations are non-dimensionalized.

The following substitutions are made:

$$v = v_0 \left(\frac{v}{v_0} \right), \quad r = R_0 \left(\frac{r}{R_0} \right), \quad z = R_0 \left(\frac{z}{R_0} \right), \quad n = n_0 \left(\frac{n}{n_0} \right) \quad (44)$$

These substitutions are performed on the parabolized conservation of cells equation (7) resulting in

$$\begin{aligned} & \left(\frac{v_0 n_0}{R_0} \right) \left(\frac{v}{v_0} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{z}{R_0} \right)} + \frac{u}{v_0} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right) + \left(\frac{n_0}{R_0^2} \right) \left(bW_c \frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right. \\ & \left. + \left(\frac{n_0}{R_0^2} \right) \left(bW_c \left(\frac{n}{n_0} \right) \left(\frac{\partial^2 C}{\partial \left(\frac{r}{R_0} \right)^2} + \frac{1}{\left(\frac{r}{R_0} \right)} \frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \right) \right) \right) \\ & = \left(\frac{n_0}{R_0^2} \right) \left(D_n \left(\frac{\partial^2 \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)^2} + \frac{1}{\left(\frac{r}{R_0} \right)} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right) \right) \end{aligned} \quad (45)$$

Equation (45) is divided by $D_n \left(\frac{n_0}{R_0^2} \right)$, yielding

$$\begin{aligned}
& \left(\frac{v_0 R_0}{D_n} \right) \left(\frac{v}{v_0} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{z}{R_0} \right)} + \frac{u}{v_0} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right) \\
& + \frac{bW_c}{D_n} \left(\frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} + \left(\frac{n}{n_0} \right) \left(\frac{\partial^2 C}{\partial \left(\frac{r}{R_0} \right)^2} + \frac{1}{\left(\frac{r}{R_0} \right)} \frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \right) \right) \\
& = \left(\frac{\partial^2 \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)^2} + \frac{1}{\left(\frac{r}{R_0} \right)} \frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right)
\end{aligned} \tag{46}$$

The substitutions (44) are preformed on the parabolized conservation of oxygen equation (11) yielding:

$$\frac{v_0}{R_0} \left(\frac{v}{v_0} \frac{\partial C}{\partial \left(\frac{z}{R_0} \right)} + \frac{u}{v_0} \frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \right) = \frac{1}{R_0^2} D_c \left(\frac{\partial^2 C}{\partial \left(\frac{r}{R_0} \right)^2} + \frac{1}{\left(\frac{r}{R_0} \right)} \frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \right) - \frac{\gamma_0 n_0}{\Delta C} \frac{n}{n_0} \tag{47}$$

Dividing both sides of Eq. (47) by $\frac{D_c}{R_0^2}$ results in:

$$\frac{v_0 R_0}{D_c} \left(\frac{v}{v_0} \frac{\partial C}{\partial \left(\frac{z}{R_0} \right)} + \frac{u}{v_0} \frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \right) = \left(\frac{\partial^2 C}{\partial \left(\frac{r}{R_0} \right)^2} + \frac{1}{\left(\frac{r}{R_0} \right)} \frac{\partial C}{\partial \left(\frac{r}{R_0} \right)} \right) - \frac{\gamma_0 n_0 R_0^2}{D_c \Delta C} \frac{n}{n_0} \quad (48)$$

Substitutions (44) are performed on Eq. (28), and the parabolized combined momentum equation is represented as:

$$\frac{\mu}{K} \frac{v_0}{R_0} \left(\frac{\partial \left(\frac{v}{v_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right) - \frac{n_0}{R_0} \left(\frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right) \theta \Delta \rho g = 0 \quad (49)$$

Dividing Eq. (49) by $\frac{\mu}{K} \frac{v_0}{R_0}$ yields:

$$\left(\frac{\partial \left(\frac{v}{v_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right) - \left(\frac{\partial \left(\frac{n}{n_0} \right)}{\partial \left(\frac{r}{R_0} \right)} \right) \frac{\theta \Delta \rho g n_0 K}{\mu v_0} = 0 \quad (50)$$

The continuity equation (30) is similarly non-dimensionalized by making substitutions (44)

and dividing by $\frac{v_0}{R_0}$ which yields:

$$\frac{1}{\left(\frac{r}{R_0} \right)} \frac{\partial \left(\left(\frac{r}{R_0} \right) \left(\frac{u}{v_0} \right) \right)}{\partial \left(\frac{r}{R_0} \right)} + \frac{\partial \left(\frac{v}{v_0} \right)}{\partial \left(\frac{z}{R_0} \right)} = 0 \quad (51)$$

The following dimensionless parameters are defined as:

$$\begin{aligned}\bar{v} &= \frac{v}{v_0}, \quad \bar{r} = \frac{r}{R_0}, \quad \bar{z} = \frac{z}{R_0}, \quad \bar{n} = \frac{n}{n_0}, \quad \bar{\gamma} = \frac{\gamma_0 R_0^2}{D_c} \frac{n_0}{\Delta C} \\ Pe_0 &= \frac{v_0 R_0}{D_c}, \quad Pe_n = \frac{v_0 R_0}{D_n}, \quad \bar{u} = \frac{u}{v_0}, \quad Pe = \frac{W_c b}{D_n}, \quad \alpha = \frac{\theta \Delta \rho g n_0 K}{\mu v_0}\end{aligned}\tag{52}$$

Using the dimensionless parameters (52), the governing equations can be presented in the following dimensionless forms.

The parabolized oxygen conservation equation may be recast as:

$$Pe_0 \left(\bar{v} \frac{\partial C}{\partial \bar{z}} + \bar{u} \frac{\partial C}{\partial \bar{r}} \right) = \frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} - \bar{\gamma} \bar{n}\tag{53}$$

It should be noted that the term $Pe_0 = \frac{v_0 R_0}{D_c}$ is the oxygen related Peclet number; it represents the ratio of strengths of the convection of oxygen to the diffusion of oxygen. The term $\bar{\gamma}$ represents the strength of oxygen consumption by the cells.

The parabolized cell conservation equation may be recast as:

$$Pe_n \left(\bar{v} \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right) + Pe \left[\frac{\partial C}{\partial \bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} + \bar{n} \left(\frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} \right) \right] = \frac{\partial^2 \bar{n}}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}}\tag{54}$$

In Eq. (54), the term associated with convection is $Pe_n = \frac{v_0 R_0}{D_n}$, the cell related Peclet number. It represents the relative strengths of cell transport by convection to cell transport by diffusion. The Peclet number associated with cell swimming along the oxygen gradient is $Pe = \frac{W_c b}{D_n}$, which shows the ratio of cell transport due to cell swimming to cell transport by diffusion.

The parabolized combined momentum equation can be presented in dimensionless form as:

$$\frac{\partial \bar{v}}{\partial \bar{r}} - \frac{\partial \bar{n}}{\partial \bar{r}} \alpha = 0.\tag{55}$$

In this equation the term $\alpha = \frac{\theta \Delta \rho g n_0 K}{\mu N_0}$ (which may be written $\frac{(\theta \Delta \rho g n_0)}{\left(\frac{\mu}{K} v_0\right)}$) shows the ratio of

the buoyancy force resulting from the density gradient to the resisting force resulting from the porous medium.

The continuity equation may be recast as:

$$\frac{1}{\bar{r}} \frac{\partial(\bar{r} \bar{u})}{\partial \bar{r}} + \frac{\partial \bar{v}}{\partial \bar{z}} = 0 \quad (56)$$

Equations (53)-(56) must be solved subject the following dimensionless boundary conditions:

at $\bar{r} = 0$:

$$\frac{\partial \bar{n}}{\partial \bar{r}} = 0, \quad \frac{\partial C}{\partial \bar{r}} = 0, \quad \bar{u} = 0, \quad \frac{\partial \bar{v}}{\partial \bar{r}} = 0 \quad (57)$$

at $\bar{r} \rightarrow \infty$:

$$\bar{n} \rightarrow 0, \quad C \rightarrow 1, \quad \bar{v} \rightarrow 0 \quad (58)$$

and the following inlet conditions:

$$\bar{z} = 0, \quad 0 \leq \bar{r} \leq 1: \quad \bar{v} = 1 \quad (59)$$

$$\bar{z} = 0, \quad \bar{r} > 1: \quad \bar{v} = 0 \quad (60)$$

The dimensionless radial velocity at the inlet is zero:

$$\bar{z} = 0: \quad \bar{u} = 0 \quad (61)$$

It is also necessary to prescribe value of dimensionless cell concentration at the inlet:

$$\bar{z} = 0: \quad \bar{n} = 1 \quad (62)$$

Dimensionless integral condition

The integral condition (39) is also non-dimensionalized by implementing substitutions (44); this results in:

$$Q = 2\pi v_0 n_0 R_0^2 \int_0^\infty \frac{r}{R_0} \frac{v}{v_0} \frac{n}{n_0} d\left(\frac{r}{R_0}\right) = constant \quad (63)$$

using Eq. (38), which states that the cell flux is constant for all z , and substituting the inlet values of cell flux, Eq. (21): $Q = \pi R_0^2 n_0 v_0$, into Equation (63) results in:

$$\pi v_0 n_0 R_0^2 = 2\pi v_0 n_0 R_0^2 \int_0^\infty \overline{r v n} d\bar{r} = constant \quad (64)$$

or,

$$\frac{1}{2} = \int_0^\infty \overline{r v n} d\bar{r} \text{ for any } \bar{z}. \quad (65)$$

Integral condition (65) is utilized in numerical integration to verify the accuracy of the computations at all depth levels.

Induced Free Stream Velocity

The situation prescribed by the inlet boundary conditions has similar properties to those of axisymmetrical laminar jet mixing of incompressible fluid. In this case a cell rich jet of radius R_0 is introduced into a cell free porous medium. As suggested by Pai and Hsieh [11], the numerical handling of such an arrangement is realized by adding a very small free stream

velocity over the entire domain of the system. The free stream downward velocity is defined as V_0 , where $V_0 = (0.03)v_0$, and is represented in dimensionless terms as : $\bar{V}_0 = \frac{V_0}{v_0}$. The free stream velocity is introduced to the dimensionless governing equations simply by replacing v with $V_0 + v$.

The dimensionless oxygen conservation equation (54) may be written as:

$$Pe_0 \left((\bar{V}_0 + \bar{v}) \frac{\partial C}{\partial \bar{z}} + \bar{u} \frac{\partial C}{\partial \bar{r}} \right) = \frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} - \bar{\gamma} \bar{n} \quad (66)$$

Dimensionless cell conservation (54) may be recast:

$$Pe_n \left((\bar{V}_0 + \bar{v}) \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right) + Pe \left[\frac{\partial C}{\partial \bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} + \bar{n} \left(\frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} \right) \right] = \frac{\partial^2 \bar{n}}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} \quad (67)$$

The momentum and continuity equations (55) and (56) are unaffected.

The dimensionless integral condition (63) and Eq. (43) are now written as

$$Q = 2\pi v_0 n_0 R_0^2 \int_0^\infty \bar{r} \bar{v} \bar{n} d\bar{r} = constant \quad (68)$$

$$Q = \pi R_0^2 n_0 (v_0 + V) \quad (69)$$

respectively.

Equating Eq. (68) to Eq. (69) yields:

$$\frac{\pi R_0^2 n_0 (v_0 + V)}{2\pi v_0 n_0 R_0^2} = \int_0^\infty \bar{r} \bar{v} \bar{n} d\bar{r} \quad (70)$$

or

$$\frac{(1 + \bar{V})}{2} = \int_0^\infty \bar{r} \bar{v} \bar{n} d\bar{r} . \quad (71)$$

Equation (41) is now used to check the accuracy of the computations.

Axial Velocity – Cell Concentration Relation

A relation between the axial velocity, v , and cell concentration, n , is used to simplify the solution procedure. This relation is found by integrating the momentum equation in parabolic form (24) with respect to r :

$$\int \frac{\mu}{K} \frac{\partial v}{\partial r} dr = \int \theta \Delta \rho g \frac{\partial n}{\partial r} dr \quad (72)$$

which results in:

$$\frac{\mu}{K} v = \theta \Delta \rho g n + c(z) \quad (73)$$

By imposing the boundary condition (10) as $r \rightarrow \infty : n \rightarrow 0, v \rightarrow 0$, it is found that:

$$c(z) = 0 \quad (74)$$

And the Eq. (73) is rewritten as:

$$\frac{\mu}{K} v = \theta \Delta \rho g n \quad (75)$$

Using the inlet conditions which state that at $z = 0, r \leq R : v = v_0, n = n_0$, Eq. (75) may be restated as:

$$\frac{\mu}{K} v_0 = \theta \Delta \rho g n_0 \quad (76)$$

or

$$1 = \frac{\theta \Delta \rho g n_0 K}{\mu v_0} \quad (76b)$$

And the dimensionless parameter $\alpha = \frac{\theta \Delta \rho g n_0 K}{\mu v_0}$ is set to unity. It appears that the

assumptions made in the formation of the parabolized governing equations are valid as long

as the condition that the buoyancy forces are perfectly balanced by the resisting forces offered by the porous medium. If this is plausible then it seems that the flow is truly governed by the medium porosity; for a specific value of porosity, there is a specific corresponding value of surface cell concentration that enables bioconvection.

Condition (76b) may be reasserted by integrating the dimensionless parabolized momentum equation (55) with respect to $\bar{r}$:

$$\int \frac{\partial \bar{v}}{\partial \bar{r}} d\bar{r} = \alpha \int \frac{\partial \bar{n}}{\partial \bar{r}} d\bar{r}$$

which results in:

$$\bar{v} = \alpha \bar{n} + c(\bar{z}) \quad (77)$$

By imposing the boundary condition (58) $\bar{r} \rightarrow \infty : \bar{n} \rightarrow 0, \bar{v} \rightarrow 0$, it is found that

$$c(\bar{z}) = 0 \quad (78)$$

Equation (77) is now presented as:

$$\bar{v} = \alpha \bar{n} \quad (79)$$

Using the dimensionless inlet conditions (which state at $z = 0, \bar{r} \leq 1 : \bar{v} = 1, \bar{n} = 1$), it is evident that again $\alpha = 1$.

The result of setting α to unity yields the relation:

$$\bar{v} = \bar{n} \quad (80)$$

It should be noted that the use of Eq. (80) creates a non-linearity in the conservation of cells

equation's convective term, $Pe_n \left((\bar{V}_0 + \bar{v}) \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right)$, which may be rewritten :

$$Pe_n \left((\bar{V}_0 + \bar{n}) \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right) \quad (81)$$

Similarity Solution

A similarity solution of the plume is also found. In order to confirm the output of the numerical solution, the resulting data of both similarity and numerical solutions will be plotted together for comparison.

The similarity solution requires symmetry in order to transform the governing equations. As it is presented in Eq (53), the conservation of oxygen equation lacks symmetry in dimensionless cell concentration. In order to produce the required symmetry, the oxygen consumption term is assumed proportional to cell concentration: $\bar{\gamma} \propto \bar{n}$.

The dimensionless parabolized oxygen conservation equation is rewritten as:

$$Pe_0 \left(\bar{v} \frac{\partial C}{\partial \bar{z}} + \bar{u} \frac{\partial C}{\partial \bar{r}} \right) = \frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} - \bar{\gamma} \bar{n}^2 \quad (82)$$

The parabolized non-dimensional governing equations are recalled for convenience.

The dimensionless parabolized cell conservation equation:

$$Pe_n \left(\bar{v} \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right) + Pe \left[\frac{\partial C}{\partial \bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} + \bar{n} \left(\frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} \right) \right] = \frac{\partial^2 \bar{n}}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} \quad (54)$$

The dimensionless parabolized combined momentum equation:

$$\frac{\partial \bar{v}}{\partial \bar{r}} - \frac{\partial \bar{n}}{\partial \bar{r}} \alpha = 0 \quad (55)$$

where $\alpha = 1$

The dimensionless continuity equation:

$$\frac{1}{\bar{r}} \frac{\partial (\bar{r} \bar{u})}{\partial \bar{r}} + \frac{\partial \bar{v}}{\partial \bar{z}} = 0 \quad (56)$$

Following Kuznetsov, et al. [8,12], a similarity solution to Eqs. (82), (54), (55), (56) is investigated. Assuming that $\bar{R}$ is the plume radius, the following scaling is utilized:

$$\bar{R}\alpha\bar{z}^a, \bar{v}\alpha\bar{z}^b, \bar{n}\alpha\bar{z}^c, C\alpha\bar{z}^d, \text{ and } \bar{u}\alpha\bar{z}^{(a+b-1)} \quad (83)$$

Substituting proportionalities (83) into Eqns. (82), (54)-(56), the following solution is obtained: $a = 1, b = -1, c = -1, d = 0$. The similarity variable is defined as:

$$\eta = \frac{\bar{r}}{\bar{z}} \quad (84)$$

The self-similar variables are introduced as:

$$\bar{v} = \frac{F'(\eta)}{\bar{r}}, \quad \bar{n} = \frac{1}{\bar{z}} N(\eta), \quad C = G(\eta) \quad (85)$$

Using definitions (84) and (85) and recognizing that:

$$\begin{aligned} \frac{\partial \bar{v}}{\partial \bar{r}} &= \frac{\partial}{\partial \bar{r}} \left(\frac{F'(\eta)}{\bar{r}} \right) \\ &= -\frac{1}{\bar{r}^2} F'(\eta) + \frac{1}{\bar{r}} \frac{\partial}{\partial \eta} (F'(\eta)) \frac{\partial \eta}{\partial \bar{r}} \\ &= -\frac{1}{\bar{r}^2} F'(\eta) + \frac{1}{\bar{r}\bar{z}} F''(\eta) \end{aligned} \quad (86)$$

and

$$\begin{aligned} \frac{\partial \bar{n}}{\partial \bar{r}} &= \frac{\partial}{\partial \bar{r}} \left(\frac{1}{\bar{z}} N(\eta) \right) \\ &= \frac{1}{\bar{z}} \frac{\partial}{\partial \eta} N(\eta) \frac{\partial \eta}{\partial \bar{r}} \\ &= \frac{1}{\bar{z}^2} N'(\eta) \end{aligned} \quad (87)$$

and that $\alpha = 1$, the combined momentum equation (55) transforms to:

$$\eta N' = F'' - \frac{1}{\eta} F' \quad (88)$$

The conservation of oxygen Eq. (53) is similarly transformed to:

$$G'' + \frac{1}{\eta} (1 + Pe_0 F) G' - \bar{\gamma} N^2 = 0 \quad (89)$$

Conservation of cells, Eq. (54), transforms to :

$$N'' + \left[\frac{1}{\eta} (1 + FPe_n) - G'Pe \right] N' + \left[\frac{1}{\eta} F'Pe_n - \frac{1}{\eta} G'Pe - G''Pe \right] N = 0 \quad (90)$$

The similarity equations (88)-(90) are solved subject to the following boundary conditions, which are obtained by transforming the dimensionless boundary conditions (57), and (58):

$$\text{At } \eta = 0: \quad N' = 0, \quad G' = 0, \quad F' - \frac{F}{\eta} = 0, \quad \frac{F''}{\eta} - \frac{F'}{\eta^2} = 0 \quad (91)$$

$$\text{As } \eta \rightarrow \infty: \quad N = 0, \quad G' = 0, \quad \frac{F'}{\eta} = 0 \quad (92)$$

Equations (88)–(90) and condition (91) are singular at $\eta = 0$. To initiate the numerical similarity solution, a series solution is obtained for very small values of η . The following series expansions are assumed for $N(\eta)$, $G'(\eta)$, and $F(\eta)$:

$$N(\eta) = \sum_{i=0}^{\infty} n_i \eta^i, \quad G'(\eta) = \sum_{i=0}^{\infty} g_i \eta^i, \quad F(\eta) = \sum_{i=0}^{\infty} f_i \eta^i \quad (93)$$

Since the similarity solution is introduced for comparison purposes only, a high order of accuracy is not required, and therefore the series is only expanded up to $i=3$. The series are thus represented as:

$$\begin{aligned} N(\eta) &= n_0 + n_1 \eta + n_2 \eta^2 + n_3 \eta^3, \quad G'(\eta) = g_0 + g_1 \eta + g_2 \eta^2 + g_3 \eta^3, \\ F(\eta) &= f_0 + f_1 \eta + f_2 \eta^2 + f_3 \eta^3 \end{aligned} \quad (94)$$

using boundary conditions (91) on (94) yield the following is found:

$$n_1 = g_0 = f_0 = f_1 = f_3 = 0 \quad (95)$$

Using an algebraic software package, Eqns. (94) and (95) are substituted into Eqns. (88)-(90), and the solutions are obtained in terms of n_1 and f_2 as:

$$F = f_2 \eta^2 - \frac{1}{4} n_0 \text{Pe} \left(\frac{f_2 \text{Pe}_n}{2\text{Pe}} - \frac{n_0^2 \bar{\gamma}}{4} \right) \eta^4 \quad (96)$$

$$N = n_0 - n_0 \text{Pe} \left(\frac{f_2 \text{Pe}_n}{2\text{Pe}} - \frac{n_0^2 \bar{\gamma}}{4} \right) \eta^2 \quad (97)$$

$$G = \frac{n_0^2 \bar{\gamma}}{4} \eta^2 + \frac{\frac{1}{2} n_0 \text{Pe} \left(\frac{f_2 \text{Pe}_n}{2\text{Pe}} - \frac{n_0^2 \bar{\gamma}}{4} \right) \frac{n_0^2 \bar{\gamma}}{4} \text{Pe}_0 + (n_0 \text{Pe})^2 \left(\frac{f_2 \text{Pe}_n}{2\text{Pe}} - \frac{n_0^2 \bar{\gamma}}{4} \right)^2 \bar{\gamma}}{4 f_2 \text{Pe}_0} \eta^4 \quad (98)$$

The solutions of Eqns. (96)-(98) are evaluated for some very small value of η . Then using these values as inlet boundary values, a Runge-Kutta method is used to solve the similarity variables. The values of n_1 and f_2 are varied until boundary conditions (91) are met. A copy of the similarity solution code is provided in Appendix III. In checking between numerical and similarity solutions, the numerical solution uses the symmetric conservation of oxygen equation (82).

Computational Procedure

The numerical solution procedure used to find the plume solution is very simple. Given the parabolic nature of the plume, the system is discretized in such a way that it is layered axially. Both the parabolized dimensionless cell and oxygen conservation equations (67) and (66) are discretized in a pair of fully implicit finite difference equations. The dimensionless continuity equation (56) is discretized explicitly and is numerically integrated for radial

velocity as suggested by Anderson [13]. A detailed description of these discretizations is given in Appendix II.

As the equations are solved in a downward stepping procedure, information is fed from the preceding layer (i) and all variables at (i+1) assume the value of the preceding layer (i). Then a variable is solved for from each of the governing equation in the order: cell concentration from conservation of cells, oxygen concentration from conservation of oxygen, radial velocity from continuity. The non-linearity (81) in the conservation of cells equation is dealt with by iteration. Also an iterative procedure is used for all variables in the i+1 layer and when all the values meet a convergence criterion ($|\text{variable}_{OLD} - \text{variable}_{NEW}| \leq \delta$ where $\delta = 10^{-5}$), the procedure begins again stepping down to the next layer. If convergence has not been met, a relaxation technique is used in which:

$$\text{variable}_{NEW} = \beta \times \text{variable}_{NEW} + (1 - \beta) \times \text{variable}_{OLD}$$

where $\beta = 0.5$. A schematic algorithm of the computational procedure is provided on the following page in Fig. 2.

Fig. 2 Numerical solution algorithm

To reiterate:

- The oxygen concentration equation is solved implicitly for oxygen concentrations at level $i+1$ ($C(i+1,j)$) using previous layer values of cell concentration, axial velocity, and radial velocity ($n(i,j)$, $v(i,j)$, $u(i,j)$).
- Next the cell conservation equation is solved for $n(i+1,j)$ using $C(i+1,j)$, $v(i,j)$, $u(i,j)$, and condition (43) which states $n(i+1,j) = v(i+1,j)$. A dummy cell concentration ($np(itt, j)$) is used to handle the new nonlinearity in cell concentration which is initially set to $np(itt, j) = n(i+1, j)$. An iterative technique is used setting $np(itt+1, j) = n(itt, j)$ until the previously mentioned convergence criterion is met.
- Using condition (43) axial velocities are assigned values: $v(i+1, j) = n(i+1, j)$.
- Radial velocities are found by integrating the continuity equation using $v(i+1,j)$.
- An iterative loop using a relaxation technique is initiated until the convergence criterion is met.
- The process is brought to the next layer and repeated

Results and Discussion

Depth

The plume properties vary with depth. It is expected that the plume profile grows in the radial direction with depth. Using this expectation along with the integral condition, it is logical that the centerline magnitudes of cell concentration and axial velocity decrease with

depth. These expectations are confirmed in Fig. 3, which shows the dimensionless cell concentrations and axial velocity profiles at different depths. Cell concentration and axial velocity are highest at the center. The velocity and cell concentration at the center of the plume decrease with depth. Conversely the plume width increases with depth.

Fig. 3 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying depths
for: $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Depth effects on oxygen concentration are investigated next. Given that the cells consume oxygen, it would make sense that the oxygen concentration is inversely proportional to cell concentration at any given depth. Furthermore as depth increases, oxygen concentrations inside the plume should decrease. The computational results of the oxygen concentrations are given in Fig. 4 at various depths. As expected the oxygen concentrations inside the plume decrease with depth. The lowest oxygen concentrations correspond with the highest cell concentrations at the plume center.

Fig. 4 Dimensionless oxygen concentration, C , at varying depths

For: $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Figure 5 shows the dimensionless radial velocity at various depths. The magnitudes of the radial velocities are much smaller than corresponding axial velocities inside the plume. Radial velocities are positive inside the plume (the plume spreads and axial velocities are decreasing with depth) and negative outside the plume (cell free oxygen rich fluid enters the plume and axial velocity increases with depth). Radial velocity profile decreases in magnitude and becomes smoother with increase in depth.

Fig. 5 Dimensionless radial velocity, $\bar{u}$, at varying depths

for: $Pe_n = Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

To explain the sign of the radial velocity Eq. (56) , the continuity equation is recalled:

$$\frac{1}{\bar{r}} \frac{\partial(\bar{r}\bar{u})}{\partial\bar{r}} + \frac{\partial\bar{v}}{\partial\bar{z}} = 0 \quad (56)$$

Rearranging and integrating yields :

$$\bar{u} = -\frac{1}{\bar{r}} \int \bar{r} \frac{\partial\bar{v}}{\partial\bar{z}} d\bar{r} + \frac{\partial\bar{v}}{\partial\bar{z}} - \frac{\partial\bar{v}}{\partial\bar{z}} \quad (99)$$

Recalling the results from Fig. 3, it becomes evident that $\frac{\partial\bar{v}}{\partial\bar{z}}$ is negative inside the plume

where the magnitude of axial velocity decreases with depth, and positive in the region where the plume becomes wider with depth. This is better illustrated in Fig. 6.

Fig. 6 Axial velocity gradient in depth

This physically explains why the radial velocity is initially positive and then becomes negative as we move along the radial axis.

In order to explain the magnitude of the radial velocity profile, the gradient $\frac{\partial \bar{v}}{\partial \bar{z}}$ is plotted along side the radial velocity in Figs.7 and 8, at $\bar{z} = 2$ and $\bar{z} = 12$ respectively.

Fig. 7 Dimensionless radial velocity, $\bar{u}$, axial velocity gradient , $\frac{\partial \bar{v}}{\partial \bar{z}}$,
for: $\bar{z} = 2, Pe_n = Pe_0 = 57.5, Pe = 10, \bar{\gamma} = 0.04$

Fig. 8 dimensionless radial velocity, $\bar{u}$;axial velocity gradient , $\frac{\partial \bar{v}}{\partial \bar{z}}$,
for: $\bar{z} = 12, Pe_n = Pe_0 = 57.5, Pe = 10, \bar{\gamma} = 0.04$

Comparing Figs.7 and 8, it is evident that in shallow regions the term $\frac{\partial \bar{v}}{\partial \bar{z}}$ is much greater in magnitude than at regions far below the surface: the radial velocity has a larger magnitude near the surface than far below. As depth increases the depth related changes in axial velocity become less pronounced, and therefore the radial velocity profile tends to become smoother with increasing depth.

Oxygen consumption term, $\bar{\gamma}$

The oxygen consumption term, $\bar{\gamma}$, introduced in the dimensionless conservation of cells equation (53), represents the strength of oxygen consumption by the cells. Obviously as this term is increased, the oxygen concentration should decrease.

The effects of varying oxygen consumption term are investigated. The computational results of the effect of changing $\bar{\gamma}$ on oxygen concentration are depicted in Figs. 9 and 10.

Fig. 9 Dimensionless oxygen concentration, C , at varying $\bar{\gamma}$

for: $\bar{z} = 2$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

As expected higher values of $\bar{\gamma}$ result in lower oxygen concentrations throughout the plume.

At lower depths the effects become more pronounced as seen in Fig.10.

Fig. 10 Dimensionless oxygen concentration, C , at varying $\bar{\gamma}$,

for: $\bar{z} = 12$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

The oxygen consumption term has relatively little effect on dimensionless cell concentrations and axial velocity profiles even at shallow depths. However at lower depths, the large oxygen consumption term has an effect on the plume profile. Figure 11 shows the effect of this term at $\bar{z} = 12$.

Fig. 11 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying $\bar{\gamma}$
for: $\bar{z} = 12$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

For small magnitudes of the cell consumption term the effect on the plume profile is negligible even at lower depths. The wider profile for large $\bar{\gamma}$ reflects cell swimming along the radial oxygen gradient that results from very strong oxygen consumption by the cells.

In Fig.12, the radial velocity profile reflects the depth gradient of axial velocity at a depth of $\bar{z} = 12$. Only for the large $\bar{\gamma}$ is an effect on radial velocity noticeable.

Fig. 12 Dimensionless radial velocity, $\bar{u}$, at varying $\bar{\gamma}$
for: $\bar{z} = 12$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Cell swimming related Peclet number, Pe

The Peclet number, $Pe = \frac{W_c b}{D_n}$, shows the relative strength of cell swimming to

cell diffusivity, and it is strongly tied to the radial oxygen concentration gradient

in the conservation equation (54)

$$Pe_n \left(\bar{v} \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right) + Pe \left[\frac{\partial C}{\partial \bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} + \bar{n} \left(\frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} \right) \right] = \frac{\partial^2 \bar{n}}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} \quad (54)$$

Since cell swimming accounts for a relatively small amount of the total cell transport, and the magnitudes of the radial oxygen gradient are expected to be relatively small, it follows that only a very large change in the value of Pe could affect the plume solution. In order to see the normally small effects produced by

the cell swimming related Peclet number, its value is increased to a greatly exaggerated value of 1000. This is not to suggest that the bacteria are actually capable of propelling themselves at such an enormous speed, but rather to greatly exaggerate the swimming effects so that they may be suitably visible from the data output.

Even for the very large Pe , at shallow depths there are no visible effects on the plume profile as evident in Fig.13; this is a result of the relatively low oxygen concentration gradient at this depth.

Fig. 13 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe
for: $\bar{z} = 2$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

The results are much different at greater depths. The results of varying Pe are given in Fig.14. The lower values of the Peclet number confirm that for small values of Pe the term has relatively little influence on the plume solution. However the term with the exaggerated value shows that the cell concentration and axial velocity much more spread out and

therefore they have a much lower centerline value. The figure displays that the cells indeed swim radially outwards towards higher oxygen concentrations.

Fig. 14 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe

for: $\bar{z} = 12$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Since the smaller Pe had little influence on the plume solution, it is expected that they should not greatly affect the oxygen concentration. The effects of Pe on oxygen concentrations are shown in Figs. 15 and 16 at $\bar{z} = 2$ and $\bar{z} = 12$, respectively.

Fig. 15 Dimensionless oxygen concentration, C , at varying Pe
for: $\bar{z} = 2$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

At shallow depths there is no visible influence on the oxygen concentration.

Fig. 16 Dimensionless oxygen concentration, C , at varying Pe
for: $\bar{z} = 12$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

At greater depths, the exaggerated Pe value shows a slight outward shift in the concentration curve. This agrees with the results of the cell concentration solution.

The radial velocity effects of the cell swimming Peclet number are shown for $\bar{z} = 12$ in Fig.17. For the unexaggerated terms, the influence is negligible. The curve of the greatly exaggerated Pe reflects the outward swimming of the cells toward higher oxygen concentrations.

Fig. 17 Dimensionless radial velocity, $\bar{u}$, at varying Pe
for: $\bar{z} = 12$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Cell related Peclet number, Pe_n

The cell related Peclet number, $Pe_n = \frac{v_0 R_0}{D_n}$, shows the relative strengths of cell convection to cell diffusion, and appears in the cell conservation equation (54). A very large value of this term represents convection dominated cell transport, while for a small value of Pe_n cell diffusion dominates cell transport. It is expected, therefore that the plume profile becomes

more wide with decreasing Pe_n . This is confirmed in Figs. 18 and 19, which show the plume profile at $\bar{z} = 2$ and $\bar{z} = 8$, respectively.

Fig. 18 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_n

for: $\bar{z} = 2$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 19 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_n

for: $\bar{z} = 6$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Even at relatively shallow depths the diffusion influenced Pe_n shows a wider slower plume profile. At greater depths, in Fig.19, the large diffusive effects are more outstanding. The plot also shows a very narrow profile for convection dominated cell transport, which is reflected in large Pe_n .

Oxygen concentrations have been found to be lowest at highest cell concentrations. It is logical then that for a larger value of cell related Peclet number, which has a higher centerline cell concentration, the centerline oxygen concentration is lower. The effect of Pe_n on dimensionless oxygen concentration is represented in Figs. 20 and 21.

Fig. 20 Dimensionless oxygen concentration, C , at varying Pe_n

for: $\bar{z} = 2$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 21 Dimensionless oxygen concentration, C , at varying Pe_n

for: $\bar{z} = 6$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

The oxygen concentrations indeed have lower centerline concentrations for higher values of Pe_n . In Fig. 21, the large diffusive effects, represented by smaller Pe_n , are dramatically reflected in the lower oxygen concentration at higher dimensionless radius.

Because the axial velocity has a strong dependence on the cell related Peclet number, it is not surprising to find that radial velocity also is greatly affected by large variations in Pe_n . The dimensionless radial velocity is plotted in Figs. 22 and 23 at $\bar{z} = 2$ and $\bar{z} = 8$, respectively.

Fig. 22 Dimensionless radial velocity, $\bar{u}$, at varying Pe_n

for: $\bar{z} = 2$, $Pe_0 = 57.5$, $Pe=10$, $\bar{\gamma} = 0.04$

Fig. 23 Dimensionless radial velocity, $\bar{u}$, at varying Pe_n

for: $\bar{z} = 6$, $Pe_0 = 57.5$, $Pe=10$, $\bar{\gamma} = 0.04$

The plots of the radial velocity profiles show that dimensionless radial velocity is smallest for very high Pe_n . The large depth gradient of axial velocity, associated with diffusion

influenced Pe_n , is reflected in the larger magnitudes of the dimensionless radial velocity for low Pe_n .

Oxygen related Peclet number, Pe_o

The Peclet number associated with oxygen, $Pe_o = \frac{v_o R_o}{D_c}$, represents the relative strengths of the convection of oxygen to the diffusion of oxygen. The fact that this term appears only in the conservation of oxygen equation, (66), coupled with the previous results which show very little dependence of the plume solution on neither the oxygen consumption term nor cell transport due to the oxygen gradient (associated with Pe), it follows then that changes in Pe_o should not greatly affect the plume solution. This is investigated by varying the magnitude of Pe_o . The effects of the oxygen related Peclet number on the plume profile are plotted in Figs. 24 and 25 at $\bar{z} = 2$ and $\bar{z} = 12$, respectively. At shallow depths there is no noticeable effect. At greater depths, however, the centerline cell concentration is lower for lower values of Pe_o . Because the lower Pe_o is influenced more heavily by the diffusion of oxygen, the oxygen concentration inside the plume is not sustained primarily by convection; the cells swimming along the oxygen gradient move outward towards higher oxygen concentrations, and by the integral condition the centerline concentration drops.

Fig. 24 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_o
for: $\bar{z} = 2$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 25 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_o
for: $\bar{z} = 12$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

It is logical to assume that the concentration of oxygen is heavily influenced by the oxygen related Peclet number. Figures 26 and 27 show that lower Pe_o curves have lower oxygen concentration everywhere. With lower values of Pe_o , diffusion of oxygen becomes more important, less oxygen is convected into the plume and there is less of a mechanism to replace oxygen consumed by the cells.

Fig. 26 Dimensionless oxygen concentration, C , at varying Pe_o

for: $\bar{z} = 2$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 27 Dimensionless oxygen concentration, C , at varying Pe_o
for: $\bar{z} = 12$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Figs. 28 and 29 show how radial velocity is influenced by the oxygen related Peclet number. Given that the axial velocity profile is not greatly affected, it is not surprising to find that the radial velocity is similarly uninfluenced.

Fig. 28 Dimensionless radial velocity, $\bar{u}$, at varying Pe_o
for: $\bar{z} = 2$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 29 Dimensionless radial velocity, $\bar{u}$, at varying Pe_o
for: $\bar{z} = 12$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Similarity solution

A similarity solution of the plume was found to compare with the numerical results. The comparisons of plume profile at $\bar{z} = 2$ and $\bar{z} = 40$ are given in Figs. 28 and 29. Oxygen concentration comparisons are shown in Figs 30 and 31.

Fig. 30 Solution comparison of dimensionless cell concentration, $\bar{n}$
for: $\bar{z} = 2$ $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 31 Solution comparison of dimensionless cell concentration, $\bar{n}$
for: $\bar{z} = 40$, $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 32 Solution comparison of dimensionless oxygen concentration, C ,
for: $\bar{z} = 2$, $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 33 Solution comparison of dimensionless oxygen concentration, C ,
for: $\bar{z} = 40$, $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Figures 28-31 show that the solutions are in better at agreement greater depths. This may be explained in a brief analysis of the similarity solution. Given the singularity found at $\eta = 0$, a set of series solutions is obtained for very small values of η . For cell concentration, this series solution is given by Eq. (95):

$$N = n_0 - n_0 Pe \left(\frac{f_2 Pe_n}{2Pe} - \frac{n_0^2 \bar{\gamma}}{4} \right) \eta^2 \quad (95)$$

which, at $\eta = 0$, reduces to $N = n_0$.

Recalling the transformation (84) which says in part that $\bar{n} = \frac{1}{\bar{z}} N(\eta)$, and recognizing that

$\eta = 0$ corresponds to $\bar{r} = 0$, it follows that at $\eta = 0$

$\bar{n}(\text{centerline}) = \frac{1}{\bar{z}} n_0$. This hints to the fact that the similarity solution agrees with the

numerical solution as $\bar{n}(\text{centerline})\bar{z} = n_0$ or that the product of $\frac{\partial}{\partial \bar{z}}(\bar{n}(\text{centerline})\bar{z}) = 0$.

The product of centerline cell concentration and depth has been plotted in Fig.32. The results show that as $\bar{z}$ increases, the product slope becomes less steep. Therefore it is logical to assume that the solutions converge at very large depths.

Fig. 34 Product of dimensionless cell concentration and depth, $\bar{n}\bar{z}$, vs. $\bar{z}$

for: $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Integral condition

Integral condition (65) is utilized in numerical integration to verify the accuracy of the computations at all depth levels. Fig. 33 shows the results of the integral vs. depth. The plot shows that the value of $\int_0^{\infty} \bar{r} \bar{v} \bar{n} d\bar{r}$ is indeed constant for all $\bar{z}$.

Fig. 35 Integral condition

for: $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Induced free stream velocity

The code incorporates use of an induced free stream velocity. Although the introduction of this velocity is used to stabilize the numerical results, its use should not drastically change the results. In Figs. 34 and 35, it is evident that the free stream velocity has relatively little

impact on the plume profile at $\bar{z} = 2$ and $\bar{z} = 12$ respectively, although the profile without the velocity is slightly wider.

Fig. 36 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, with and without free stream velocity

for: $\bar{z} = 2$, $Pe = 10$, $Pen_0 = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 37 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, with and without free stream velocity

for: $\bar{z} = 12$, $Pe = 10$, $Pen_0 = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Figures 36 and 37 show that the free stream velocity has very little effect on the oxygen concentration.

Fig. 38 Dimensionless oxygen concentration, C , with and without free stream velocity

for: $\bar{z} = 2$ $Pe_n = Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 39 Dimensionless oxygen concentration, C , with and without free stream velocity

for: $\bar{z} = 12$ $Pe_n = Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

It is expected that the radial velocity is similarly unaffected by introducing the free stream velocity. This is confirmed in Figs. 38 and 39.

Fig. 40 Dimensionless radial velocity, $\bar{u}$, with and without free stream velocity
for: $\bar{z} = 2$, $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 41 Dimensionless radial velocity, $\bar{u}$, with and without free stream velocity
for: $\bar{z} = 12$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Conclusions

The results of the data output in the preceding section show that the numerical and similarity solutions agree at increasing depth. This agreement gives credibility to the numerical code.

The integral condition is met at all depths, so the accuracy of the numerical code is met. The effects of varying the dimensionless parameters make sense in the code output. This shows that the numerical code is producing logical output.

References

1. Kessler, J.O., Cooperative and concentrative phenomena of swimming microorganisms, *Contemp. Phys.*, vol. 26, pp. 147-166, 1985b.
2. Kessler, J.O., Wiseley, D.A., Remrick, K.E., Marthaler, D.E, Individual and collective dynamics of swimming bacteria, in: Schreckenburg, M., Wolf, D.E. (Eds.), *Proceedings of the Workshop "Traffic and Granular Flow '97"*, Springer, New York, 1997, pp. 37-51.
3. Kessler, J.O., Burnett, G.D., Remrick, K.E., Mutual Dynamics of swimming microorganisms and their fluid habitat, in: Sorensen, M.P., Scott, A.C. (Eds.), *Nonlinear Science at the Dawn of the 21st Century*, Christiansen, P.L., Springer, New York, 2000, pp. 409-426.
4. Harashima, A., Watanabe, M., Fujishiro, I., Evolution of bioconvection patterns in a culture of motile flagellates, *Phys. Fluids* 31 (1988) 764-775.
5. Kessler, J.O., Turbulence, Mixing, and Dynamics of Bacterial Suspensions, *Presentation at the ICTAM 2000*, Chicago, Illinois, August 27 – September 2, 2000.
6. Metcalfe, M., Pedley, T., J. Falling plumes in bacterial bioconvection, *J. Fluid Mech.* (2001), vol 445 pp.121-149.

7. Hillesdon, A.J., Pedley, T., J., Kessler, J.O., The development of concentration gradients in a suspension of chemotactic bacteria, *Bull. Math. Biol.* 57 (1995) 299-344
8. Kuznetsov, A.V., Avramenko, A.A., Geng, P., Analytical Investigation of a Falling Plume Caused by Bioconvection of Oxytactic Bacteria in a Fluid Saturated Porous Medium, *International Journal of Engineering Science*, in press, 2003.
9. Kessler, J.O. 1986 The external dynamics of swimming micro-organisms. *Progress in Phycological Research* 4, Biopress, Bristol, 257-307
10. Darcy, H.P., *Les Fontaines Publiques de la Ville de Dijon*, Victor Dalmont, Paris (1856).
11. Pai, S. I., Hsieh, T., Numerical Solution of Laminar Jet Mixing With and Without Free Stream, *Appl. Sci. Res.*(1972), vol 27.
12. Kuznetsov, A.V., Avramenko, A.A., Geng, P., A similarity solution for a falling plume in bioconvection of oxytactic bacteria in a porous medium, *Int. Commun. Heat Mass Transfer* 30 (2003) 37-46.
13. Anderson, D. A., Tannenhill, J. C., Pletcher, R. H., *Computational Fluid Mechanics and Heat Transfer*, Hemisphere, 1984.

Appendices

APPENDIX I –Figures

Figures not displayed in the Results and Discussion section are presented here. These figures show parameter effects on the plume solution and compare solution results at depth levels that were not included in the Results and Discussion section.

Figures 42-50 show effects of consumption term, $\bar{\gamma}$

Figures 51-56 show effects of cell swimming related Peclet number, Pe

Figures 57-62 show effects of cell related Peclet number, Pe_n

Figures 63-68 show effects of induced free stream velocity

Figures 69-74 show effects of cell related Peclet number, Pe_o

Fig. 42 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying $\bar{\gamma}$,

for: $\bar{z} = 2$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 43 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying $\bar{\gamma}$,

for: $\bar{z} = 6$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 44 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying $\bar{\gamma}$,
for: $\bar{z} = 8$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 45 Dimensionless oxygen concentration, C , at varying $\bar{\gamma}$,
for: $\bar{z} = 6$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 46 Dimensionless oxygen concentration, C , at varying $\bar{\gamma}$,
for: $\bar{z} = 8$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 47 Dimensionless radial velocity, $\bar{u}$, at varying $\bar{\gamma}$,
for: $\bar{z} = 2$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 48 Dimensionless radial velocity, $\bar{u}$, at varying $\bar{\gamma}$,
for: $\bar{z} = 6$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 49 Dimensionless radial velocity, $\bar{u}$, at varying $\bar{\gamma}$,
for: $\bar{z} = 8$, $Pe_n = Pe_0 = 57.5$, $Pe = 10$

Fig. 50 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe
for: $\bar{z} = 6$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 51 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe
for: $\bar{z} = 8$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 52 Dimensionless oxygen concentration, C , at varying Pe
for: $\bar{z} = 6$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 53 Dimensionless oxygen concentration, C , at varying Pe
for: $\bar{z} = 8$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 54 Dimensionless radial velocity, $\bar{u}$, at varying Pe
for: $\bar{z} = 2$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 55 Dimensionless radial velocity, $\bar{u}$, at varying Pe
for: $\bar{z} = 6$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 56 Dimensionless radial velocity, $\bar{u}$, at varying Pe
for: $\bar{z} = 8$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 57 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_n
for: $\bar{z} = 8$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 58 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_n
for: $\bar{z} = 12$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 59 Dimensionless oxygen concentration, C , at varying Pe_n
for: $\bar{z} = 8$, $Pe_0 = 57.5$, $Pe = 10$ $\bar{\gamma} = 0.04$

Fig. 60 Dimensionless oxygen concentration, C , at varying Pe_n
for: $\bar{z} = 12$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 61 Dimensionless radial velocity, $\bar{u}$, at varying Pe_n

for: $\bar{z} = 8$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 62 Dimensionless radial velocity, $\bar{u}$, at varying Pe_n

for: $\bar{z} = 12$, $Pe_0 = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 63 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, with and without free stream velocity

for: $\bar{z} = 6$, $Pe = 10$, $Pen_0 = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 64 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, with and without free stream velocity

for: $\bar{z} = 8$, $Pe = 10$, $Pen_0 = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 65 Dimensionless oxygen concentration, C , with and without free stream velocity

for: $\bar{z} = 6$, $D_c = D_n = 1.9 \times 10^{-8} \text{ m}^2/\text{s}$, $Pe = 10$, $Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 66 Dimensionless oxygen concentration, C , with and without free stream velocity

for: $\bar{z} = 8$ $D_c = D_n = 1.9 \times 10^{-8} \text{ m}^2/\text{s}$, $Pe = 10$, $Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 67 Dimensionless radial velocity, $\bar{u}$, with and without free stream velocity

for: $\bar{z} = 6$, $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 68 Dimensionless radial velocity, $\bar{u}$, with and without free stream velocity
for: $\bar{z} = 8$, $Pe = 10$, $Pe_n = Pe_0 = 57.5$, $\bar{\gamma} = 0.04$

Fig. 69 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_o
for: $\bar{z} = 6$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 70 Dimensionless cell concentration, $\bar{n}$, dimensionless axial velocity, $\bar{v}$, at varying Pe_o
for: $\bar{z} = 8$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 71 Dimensionless oxygen concentration, C , at varying Pe_o

for: $\bar{z} = 6$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 72 Dimensionless oxygen concentration, C , at varying Pe_o

for: $\bar{z} = 8$, $Pe_n = 57.5$, $Pe = 10$, $\bar{\gamma} = 0.04$

Fig. 73 Dimensionless radial velocity, $\bar{u}$, at varying Pe_o

for: $\bar{z} = 6$, $Pe_n = 57.5$, $Pe=10$, $\bar{\gamma} = 0.04$

Fig. 74 Dimensionless radial velocity, $\bar{u}$, at varying Pe_o

for: $\bar{z} = 8$, $Pe_n = 57.5$, $Pe=10$, $\bar{\gamma} = 0.04$

APPENDIX II -Discretization

The discretization is forward-differenced for first order radial and axial derivatives, and central difference for second order radial derivatives. Non-varying step sizes are used in both axial and radial directions.

The non-dimensional parabolized conservation of oxygen equation with induced free stream velocity (66),

$$Pe_0 \left((\bar{V}_0 + \bar{v}) \frac{\partial C}{\partial \bar{z}} + \bar{u} \frac{\partial C}{\partial \bar{r}} \right) = \frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} - \bar{\gamma} \bar{n}$$

is represented in discrete form as:

$$Pe_0 \left((\bar{V}_0 + \bar{v}_j^{i+1}) \frac{C_j^{i+1} - C_j^i}{\Delta \bar{z}} + \bar{u}_j^{i+1} \frac{C_j^{i+1} - C_{j-1}^{i+1}}{\Delta \bar{r}} \right) = \frac{C_{j+1}^{i+1} - 2C_j^{i+1} + C_{j-1}^{i+1}}{\Delta \bar{r}^2} + \frac{1}{\bar{r}_j} \frac{C_j^{i+1} - C_{j-1}^{i+1}}{\Delta \bar{r}} - \bar{\gamma} \bar{n}_j^{i+1}$$

or

$$\begin{aligned} & C_{j+1}^{i+1} \left(-\frac{1}{\Delta \bar{r}^2} \right) \\ & + C_j^{i+1} \left(Pe_0 \left(\frac{(\bar{V}_0 + \bar{v}_j^{i+1})}{\Delta \bar{z}} + \frac{\bar{u}_j^{i+1}}{\Delta \bar{r}} \right) + \frac{2}{\Delta \bar{r}^2} - \frac{1}{\bar{r}_j} \frac{1}{\Delta \bar{r}} \right) \\ & + C_{j-1}^{i+1} \left(-Pe_0 \frac{\bar{u}_j^{i+1}}{\Delta \bar{r}} - \frac{2}{\Delta \bar{r}^2} + \frac{1}{\bar{r}_j} \frac{1}{\Delta \bar{r}} \right) \\ & = Pe_0 (\bar{V}_0 + \bar{v}_j^{i+1}) \frac{C_j^i}{\Delta \bar{z}} - \bar{\gamma} \bar{n}_j^{i+1} \end{aligned}$$

Of course, the coefficients of cell concentrations on the left hand side correspond to the diagonalized entries.

The conservation of cells equation is similarly discretized. It should be noted that the non-linearity in the convective term (81) is not represented as in Eq. (81), which states:

$$Pe_0 \frac{D_c}{D_n} \left((\bar{V}_0 + \bar{n}) \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right)$$

Instead, the parabolized dimensionless cell conservation equation with induced free stream velocity (67) ,

$$Pe_0 \frac{D_c}{D_n} \left((\bar{V}_0 + \bar{v}) \frac{\partial \bar{n}}{\partial \bar{z}} + \bar{u} \frac{\partial \bar{n}}{\partial \bar{r}} \right) + Pe \left[\frac{\partial C}{\partial \bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}} + \bar{n} \left(\frac{\partial^2 C}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial C}{\partial \bar{r}} \right) \right] = \frac{\partial^2 \bar{n}}{\partial \bar{r}^2} + \frac{1}{\bar{r}} \frac{\partial \bar{n}}{\partial \bar{r}}$$

is used and the computation of cell concentration is iterated until

$$|\bar{n} - \bar{v}| \leq \beta \text{ or } |\bar{n}_j^{i+1} - \bar{v}_j^{i+1}| \leq \beta \text{ for all } j.$$

Equation (67) is written in discrete form as:

$$\begin{aligned} & Pe_0 \frac{D_c}{D_n} \left((\bar{V}_0 + \bar{v}_j^{i+1}) \frac{\bar{n}_j^{i+1} - \bar{n}_j^i}{\Delta \bar{z}} + \bar{u}_j^{i+1} \frac{\bar{n}_j^{i+1} - \bar{n}_{j-1}^{i+1}}{\Delta \bar{r}} \right) \\ & + Pe \left[\frac{C_j^{i+1} - C_{j-1}^{i+1}}{\Delta \bar{r}} \frac{\bar{n}_j^{i+1} - \bar{n}_{j-1}^{i+1}}{\Delta \bar{r}} + \bar{n}_j^{i+1} \left(\frac{C_{j+1}^{i+1} - 2C_j^{i+1} + C_{j-1}^{i+1}}{\Delta \bar{r}^2} + \frac{1}{\bar{r}_j} \frac{C_j^{i+1} - C_{j-1}^{i+1}}{\Delta \bar{r}} \right) \right] \\ & - \frac{\bar{n}_{j+1}^{i+1} - 2\bar{n}_j^{i+1} + \bar{n}_{j-1}^{i+1}}{\Delta \bar{r}^2} + \frac{1}{\bar{r}_j} \frac{\bar{n}_j^{i+1} - \bar{n}_{j-1}^{i+1}}{\Delta \bar{r}} = 0 \end{aligned}$$

or as

$$\begin{aligned}
& \bar{n}_{j+1}^{i+1} \left(-\frac{1}{\Delta \bar{r}^2} \right) \\
& + \bar{n}_j^{i+1} \left(Pe_0 \frac{D_c}{D_n} \left(\frac{(\bar{V}_0 + \bar{V}_j^{i+1})}{\Delta \bar{z}} + \frac{\bar{u}_j^{i+1}}{\Delta \bar{r}} \right) + Pe \left[\frac{C_j^{i+1} - C_{j-1}^{i+1}}{\Delta \bar{r}^2} + \left(\frac{C_{j+1}^{i+1} - 2C_j^{i+1} + C_{j-1}^{i+1}}{\Delta \bar{r}^2} + \frac{1}{\bar{r}_j} \frac{C_j^{i+1} - C_{j-1}^{i+1}}{\Delta \bar{r}} \right) \right] + \frac{2}{\Delta \bar{r}^2} - \frac{1}{\bar{r}_j} \frac{1}{\Delta \bar{r}} \right) \\
& + \bar{n}_{j-1}^{i+1} \left(-Pe_0 \frac{D_c}{D_n} \frac{\bar{u}_j^{i+1}}{\Delta \bar{r}} - Pe \frac{C_j^{i+1} - C_{j-1}^{i+1}}{\Delta \bar{r}^2} - \frac{1}{\Delta \bar{r}^2} + \frac{1}{\bar{r}_j} \frac{1}{\Delta \bar{r}} \right) \\
& = Pe_0 \frac{D_c}{D_n} \frac{(\bar{V}_0 + \bar{V}_j^{i+1})}{\Delta \bar{z}}
\end{aligned}$$

Tri-diagonalized Matrix entries:

If $f=1$ corresponds to $r = 1$ ($j=2$), and the number of discretized points - 2 = p ,

$$\begin{bmatrix}
B(1) & D(1) & 0 & 0 & 0 & \dots & \dots & 0 \\
A(2) & B(2) & D(2) & 0 & 0 & \dots & \dots & 0 \\
0 & A(3) & B(3) & D(3) & 0 & \dots & \dots & 0 \\
\dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\
0 & \dots & \dots & 0 & A(p-2) & B(p-2) & D(p-2) & 0 \\
0 & \dots & \dots & 0 & 0 & A(p-1) & B(p-1) & D(p-1) \\
0 & \dots & \dots & 0 & 0 & 0 & A(p) & B(p)
\end{bmatrix} x = \begin{bmatrix} C(1) \\ C(2) \\ C(3) \\ \dots \\ C(p-2) \\ C(p-1) \\ C(p) \end{bmatrix} = \begin{bmatrix} K(1) \\ K(2) \\ K(3) \\ \dots \\ K(p-2) \\ K(p-1) \\ K(p) \end{bmatrix}$$

is used to solve for variables C .

The dimensionless continuity equation (6)

$$\frac{1}{\bar{r}} \frac{\partial(\bar{r} \bar{u})}{\partial \bar{r}} + \frac{\partial \bar{v}}{\partial \bar{z}} = 0$$

is rearranged as:

$$\frac{\partial(\bar{r} \bar{u})}{\partial \bar{r}} = -\bar{r} \frac{\partial \bar{v}}{\partial \bar{z}}$$

and integrated by separation of variables

$$\int \partial(\bar{r} \bar{u}) = \int \left(-\bar{r} \frac{\partial \bar{v}}{\partial \bar{z}} \right) \partial \bar{r}$$

which results in:

$$\bar{r} \bar{u} = \int \left(-\bar{r} \frac{\partial \bar{v}}{\partial \bar{z}} \right) \partial \bar{r}$$

Using trapezoidal rule for integration :

$$\bar{r} \bar{u} = \frac{\Delta \bar{r}}{2} \sum_{j=1}^p \left(\bar{r} \frac{\partial \bar{v}}{\partial \bar{z}}(j-1) + \bar{r} \frac{\partial \bar{v}}{\partial \bar{z}}(j) \right)$$

And discretizing yields:

$$\bar{r}_j \bar{u}_j^i = \frac{\Delta \bar{r}}{2} \sum_{j=2}^p \left(\bar{r}_{j-1} \frac{\bar{v}_{j-1}^{i+1} - \bar{v}_{-1j}^i}{\Delta \bar{z}} + \bar{r}_j \frac{\bar{v}_j^{i+1} - \bar{v}_j^i}{\Delta \bar{z}} \right)$$

APPENDIX III – Code

Codes of the two solution types used in this thesis are provided here.

Numerical Solution Code

```
program impbioconv
integer, parameter::dp=selected_real_kind(15,99)
real(kind=dp):: dr,dz
real(kind=dp):: r,z
real(kind=dp), dimension(2,20001)::u,v,c,n
real(kind=dp), dimension(19999)::A,B,D,K,x
real(kind=dp)::pe,pe0,alpha,gamma,dc,dn,int,v0,min,g,q
integer::i,j,m,p,itt,num,nl,depth,dum,lup
real(kind=dp)::beta,betac,betan,betav,betau
real(kind=dp), dimension(20001)::uold,vold,cold,nold

open(unit=14,file="intrvn250.dat",status="unknown")
open(unit=15,file="nz.dat",status="unknown")
open(unit=16,file="c200k.dat",status="unknown")
open(unit=17,file="n200k.dat",status="unknown")
open(unit=18,file="u200k.dat",status="unknown")
open(unit=19,file="c400k.dat",status="unknown")
open(unit=20,file="n400k.dat",status="unknown")
open(unit=21,file="u400k.dat",status="unknown")

p=20001
m=2
nl=19999
dr=.001_dp
dz=.0001_dp

g=.5

v0=3.D-2
dc=1.9D-9
dn=dc
pe=10.D0
pe0=57.50
alpha=1.D0
gamma=4.D-2
min=1.D-5

z=0d0
num=1
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!! inlet condition values are assigned to first layer and second!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
i=1
do j=1,1001
u(i,j)=0.
v(i,j)=1.D0
n(i,j)=1.D0
c(i,j)=1.D0
```

```

end do
do j= 1002,p
  u(i,j)=0.
  v(i,j)=0.
  n(i,j)=0.
  c(i,j)=1.D0
end do

i=1

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! integral condition check for first layer!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

call intrvn(dr,v,n,i,m,p,int,v0)
write(*,*)z,int

i=2

Do j=2,p
  u(i,j)=u(i-1,j)
  v(i,j)=v(i-1,j)
  n(i,j)=n(i-1,j)
  c(i,j)=c(i-1,j)
end do
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! how far to move down- axial stepping !!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
do depth=2,400002
  z=depth*dz
  itt=0.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!assign previous layers values!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
  Do j=1,p
    u(i-1,j)=u(i,j)
    v(i-1,j)=v(i,j)
    n(i-1,j)=n(i,j)
    c(i-1,j)=c(i,j)
  end do
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! set up vals to be compared with from old to updated itter#1 vals!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

call oxy(pe0,gamma,m,p,dr,dz,A,B,D,K,c,n,v,u,i,v0,nl)
call tridiag(A,B,D,x,K,nl)
do j=1,p-2
  c(i,j+1)=x(j)
end do
c(i,1)=c(i,2)
c(i,p)=c(i,p-1)

```



```

do j=1,p
  v(i,j)=n(i,j)
end do
do
  call cell(dc,dn,pe,pe0,m,p,dr,dz,A,B,D,K,c,n,v,u,i,v0,nl)
  call tridiag(A,B,D,x,K,nl)
  do j=1,p-2
    n(i,j+1)=x(j)
  end do
  n(i,1)=n(i,2)
  n(i,p)=0

  q=abs(v(i,1)-n(i,1))
  do j=2,p
    q2=abs(v(i,j)-n(i,j))
    if (q.lt.q2) then
      q=q2
    end if
  end do
  if (q.le.min) exit

  call mom(alpha,i,m,p,n,v)
end do

if (depth.ge.1) then
  call cont(dr,dz,m,p,v,u,i)
end if

do j=2,p-2
  cold(j)=c(i,j)
  nold(j)=n(i,j)
  uold(j)=u(i,j)
  vold(j)=v(i,j)
end do
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!! itterate until convergence!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
do
  itt=itt+1

  call oxy(pe0,gamma,m,p,dr,dz,A,B,D,K,c,n,v,u,i,v0,nl)
  call tridiag(A,B,D,x,K,nl)
  do j=1,p-2
    c(i,j+1)=x(j)
  end do
  c(i,1)=c(i,2)
  c(i,p)=c(i,p-1)

  do j=1,p
    v(i,j)=n(i,j)
  end do
  do
    call cell(dc,dn,pe,pe0,m,p,dr,dz,A,B,D,K,c,n,v,u,i,v0,nl)

```

```

        call tridiag(A,B,D,x,K,nl)
        do j=1,p-2
            n(i,j+1)=x(j)
        end do
        n(i,1)=n(i,2)
        n(i,p)=0

        q=abs(v(i,1)-n(i,1))
        do j=2,p
            q2=abs(v(i,j)-n(i,j))
            if (q.lt.q2) then
                q=q2
            end if
        end do

        if (q.le.min) exit

        call mom(alpha,i,m,p,n,v)
    end do

    if (depth.ge.1) then
        call cont(dr,dz,m,p,v,u,i)
    end if

    call
maxdiff(i,p,m,c,n,u,v,uold,cold,nold,vold,beta,betau,betav,betan,betac)
    if (abs(beta).lt.min) exit
    call relax(i,p,m,c,n,u,v,uold,cold,nold,vold,g)
    do j=2,p-2
        cold(j)=c(i,j)
        nold(j)=n(i,j)
        uold(j)=u(i,j)
        vold(j)=v(i,j)
    end do

    end do
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!now have met convergence  check interal and move to next layer!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

    num=num+1
    dum=dum+1
    if (dum.eq.100) then

        call intrvn(dr,v,n,i,m,p,int,v0)
        write (14,*)z,int
        write (15,*)z,n(i+1,1)*z
        dum=0
    end if

    if(depth.eq.300000) then
        do j=1,p
            r=(j-1)*dr
            write(16,*) r,c(i,j)
            write(17,*)r,n(i,j)
            write(18,*)r,u(i,j)

```

```

end do
end if
if(depth.eq.400000) then
  do j=1,p
    r=(j-1)*dr
    write(19,*) r,c(i,j)
    write(20,*)r,n(i,j)
    write(21,*)r,u(i,j)
  end do
end if

```

```

end do
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! very last layer has been solved !!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

end
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
!!! oxy calculates matrix coefficients for oxygen concentration C
!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
SUBROUTINE oxy(pe0,gamma,m,p,dr,dz,A,B,D,K,c,n,v,u,i,v0,nl)
integer,intent(in)::i,m,p,nl
integer, parameter::dp=selected_real_kind(15,99)
real(kind=dp),intent(in):: dr,dz,v0
real(kind=dp), dimension(m,p),intent(in)::u,v,n,c
real(kind=dp), dimension(nl),intent(out)::A,B,D,K
real(kind=dp),intent(in)::gamma,pe0
integer::j,f

```

```

B(1)=pe0*(v(i,2)+v0)/dz+1.D0/dr/dr
D(1)=-1.D0/dr/dr
j=2
do f=2,p-3
  j=j+1
  A(f)=-(pe0*u(i,j)-1.D0/(dr*(j-1)))/dr-1.D0/dr/dr
  B(f)=-A(f)+1.D0/dr/dr+pe0*(v(i,j)+v0)/dz
  D(f)=-1.D0/dr/dr
end do
j=j+1
!A(p-2)=-(pe0*u(i,j)-1.D0/(dr*(j-1)))/dr-1.D0/dr/dr !dcdn=0@b1
!B(p-2)=-A(p-2)+pe0*v(i,j)/dz !dcdn=0@b1
A(p-2)=-(pe0*u(i,j)-1.D0/(dr*(j-1)))/dr-1.D0/dr/dr !c=1@b1
B(p-2)=-A(p-2)+1.D0/dr/dr+pe0*(v(i,j)+v0)/dz !c=1@b1

```

```

j=1
do f=1,p-2

```

```

j=j+1
K(f)= pe0*(v(i,j)+v0)/dz*c(i-1,j)&
      -gamma*n(i,j)*n(i,j)
end do
      K(p-2)=K(p-2)+1.D0/dr/dr      !c=1@b1

end subroutine oxy

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
!!! cell calculates matrix coefficients for cell concentration N
!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
subroutine cell(dc,dn,pe,pe0,m,p,dr,dz,A,B,D,K,c,n,v,u,i,v0,nl)
integer,intent(in)::i,m,p,nl
integer, parameter::dp=selected_real_kind(15,99)
real(kind=dp),intent(in):: dr,dz,v0
real(kind=dp), dimension(m,p),intent(in)::u,v,c,n
real(kind=dp), dimension(nl),intent(out)::A,B,D,K
real(kind=dp),intent(in)::pe,pe0,dc,dn
integer::j,f

B(1)=pe0*dc/dn*(v(i,2)+v0)/dz&
      +1.D0/dr/dr&
      +pe/dr/dr*(c(i,3)-c(i,2))

D(1)=-1.D0/dr/dr
j=2

do j=3,p-2

  A(j-1)=-pe0*dc/dn*u(i,j)/dr&
    -pe*(c(i,j)-c(i,j-1))/dr/dr&
    +1.D0/(dr*(j-1))/dr&
    -1.D0/dr/dr
  B(j-1)=-A(j-1)&
    +1.D0/dr/dr&
    +pe0*dc/dn*(v(i,j)+v0)/dz&
    +pe*(c(i,j+1)-2.D0*c(i,j)+c(i,j-1))/dr/dr&
    +pe*(c(i,j)-c(i,j-1))/(dr*(j-1))/dr
  D(j-1)=-1.D0/dr/dr
end do
j=p-1

A(j-1)=-pe0*dc/dn*u(i,j)/dr&
  -pe*(c(i,j)-c(i,j-1))/dr/dr&
  +1.D0/(dr*(j-1))/dr&
  -1.D0/dr/dr
B(j-1)=-A(j-1)&
  +1.D0/dr/dr&
  +pe0*dc/dn*(v(i,j)+v0)/dz&
  +pe*(c(i,j+1)-2.D0*c(i,j)+c(i,j-1))/dr/dr&
  +pe*(c(i,j)-c(i,j-1))/(dr*(j-1))/dr

```

```

j=1
do f=1,p-2
  j=j+1
  K(f)=pe0*dc/dn*(v(i,j)+v0)/dz*n(i-1,j)
end do

end subroutine cell

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
!!! mom calculates    axial velocity V from momentum!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
subroutine mom(alpha,i,m,p,n,v)
integer, parameter::dp=selected_real_kind(15,99)
integer,intent(in)::i,m,p
real(kind=dp), dimension(m,p),intent(in)::n
real(kind=dp),intent(in)::alpha
real(kind=dp), dimension(m,p),intent(out)::v
integer:: j
do j=1,p
  v(i,j)=alpha*n(i,j)
end do

end subroutine mom

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
!!! cont calculates    radial velocity u by integrating
continuity!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!
subroutine cont(dr,dz,m,p,v,u,i)
integer,intent(in)::i,m,p
integer, parameter::dp=selected_real_kind(15,99)
real(kind=dp),intent(in):: dr,dz
real(kind=dp):: int
real(kind=dp), dimension(m,p),intent(in)::v
real(kind=dp), dimension(m,p),intent(inout)::u
integer::j

int = 0.
u(i,1)=0.
do j=2,p
  int =int+dr*dr/2.D0/dz*((j-1)*(v(i,j)-v(i-1,j)))+(j-2)*(v(i,j-1)-v(i-1,j-1)))
  u(i,j)=-int/dr/(j-1)
end do

end subroutine cont

```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!! tridiag solves for the unknowns in matrix set !!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
subroutine tridiag(A,B,D,X,K,nl)
integer, parameter::dp=selected_real_kind(15,99)
integer, intent(in)::nl
real(kind=dp), dimension(nl), intent(in)::A,B,D,K
real(kind=dp), dimension(nl), intent(out)::X
real(kind=dp), dimension(nl)::gam
real(kind=dp)::bet

bet=B(1)
X(1)=K(1)/bet
do j=2,nl
  gam(j)=D(j-1)/bet
  bet=B(j)-A(j)*gam(j)
  X(j)=(K(j)-A(j)*X(j-1))/bet
end do
do j=nl-1,1,-1
  X(j)=X(j)-gam(j+1)*X(j+1)
end do
end subroutine tridiag

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!
!!! max diff finds greatest difference between iterations , names it
beta!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!
subroutine
maxdiff(i,p,m,c,n,u,v,uold,cold,nold,vold,beta,betau,betav,betan,betac)
integer,intent(in)::i,m,p
integer, parameter::dp=selected_real_kind(15,99)
real(kind=dp), dimension(m,p), intent(in)::u,v,c,n
real(kind=dp), dimension(p), intent(in)::uold,cold,nold,vold
real(kind=dp), intent(out)::beta,betav,betan,betau,betac
real(kind=dp)::diffn,diffu,diffv,diffc
integer::j

betac=0.
betan=0.
betau=0.
betav=0.
beta=0.
do j=2,p-2
  diffc=((cold(j)-c(i,j)))

  if (betac.lt.abs(diffc)) then
    betac=abs(diffc)
  end if
end do
do j=2,p-2
  diffn=abs((nold(j)-n(i,j)))
  if (betan.lt.diffn) then

```

```

        betan=diffn
    end if
end do
do j=2,p-2
    diffv=abs((vold(j)-v(i,j)))
    if (betav.lt.diffv) then
        betav=diffv
    end if
end do
do j=2,p-2
    diffu=abs((uold(j)-u(i,j)))
    if (betau.lt.diffu) then
        betau=diffu
    end if
end do

beta=0
if (beta.lt.betau) beta=betau
if (beta.lt.betav) beta=betav
if (beta.lt.betac) beta=betac
if (beta.lt.betan) beta=betan

end subroutine maxdiff

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!! intrvn is an integration subroutine for integral condition!!!!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

subroutine intrvn(dr,v,n,i,m,p,int,v0)
integer,intent(in)::i,m,p
integer, parameter::dp=selected_real_kind(15,99)
real(kind=dp), dimension(m,p),intent(in)::v,n
real(kind=dp), intent(out)::int
real(kind=dp), intent(in)::dr,v0

int=0.
do j=1,p-1
    int=int+dr/2.D0*((j-1)*dr*(v(i,j)+v0)*n(i,j)+j*dr*(v(i,j+1)+v0)*n(i,j+1))
end do

end subroutine intrvn

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
subroutine relax(i,p,m,c,n,u,v,uold,cold,nold,vold,g)
integer,intent(in)::i,m,p
integer, parameter::dp=selected_real_kind(15,99)
real(kind=dp), dimension(m,p),intent(inout)::u,v,c,n
real(kind=dp), dimension(p),intent(in)::uold,cold,nold,vold
real(kind=dp), intent(in)::g
integer::j
do j=2,p-2
    c(i,j)=g*c(i,j)+(1-g)*cold(j)
    n(i,j)=g*n(i,j)+(1-g)*nold(j)
    v(i,j)=g*v(i,j)+(1-g)*vold(j)
    u(i,j)=g*u(i,j)+(1-g)*uold(j)

```

```

end do
end subroutine relax
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

Similarity Solution Code

```

PROGRAM SIMILAR
IMPLICIT REAL*8 (A-H)
IMPLICIT REAL*8 (O-Z)
  DIMENSION WORK(39), IWORK(5), F(6)
  COMMON PE, PE_N, PE_0, GAMMA
  REAL*8 N0, NN, NN_PR
  EXTERNAL DERIVS
  OPEN(9, FILE='n40k.dat')
  OPEN(10, FILE='fl_eta40k.dat')
  OPEN(11, FILE='g140k.dat')
  OPEN(12, FILE='g40k.dat')

C INPUT PARAMETERS
  z=40D0
  COEF=1D-1

  NPOINTS=2000
  PE=10D0
  PE_N=57.5D0
  PE_0=57.5D0
  GAMMA=0.04D0

  N0=0.3811760D0*z
  F2=N0/2D0
  G0= 0.98915D0-.00007345228D0

  RELERR0=5D-12
  ABSERR0=1D-15

C PERTURBATION SOLUTION

  ETA=0.0005D0

  FF=F2*ETA*ETA-0.25D0*N0*PE*(F2*PE_N/(2D0*PE)
*   -N0*N0*GAMMA/4D0)*ETA*ETA*ETA*ETA
  FF_PR=2D0*F2*ETA-N0*PE*(F2*PE_N/(2D0*PE)
*   -N0*N0*GAMMA/4D0)*ETA*ETA*ETA

  NN=N0-N0*PE*(F2*PE_N/(2*PE)-N0*N0*GAMMA/4D0)*ETA*ETA
  NN_PR=-2D0*N0*PE*(F2*PE_N/(2*PE)-N0*N0*GAMMA/4D0)*ETA

  GG_PR=2D0*0.25D0*N0*N0*GAMMA*ETA+
*   4D0*( (0.5D0*N0*PE*(F2*PE_N/(2D0*PE)-N0*N0*GAMMA/4D0)
*   *N0*N0*GAMMA*PE_0/4D0+N0*N0*PE*PE*(F2*PE_N/(2D0*PE)-
*   N0*N0*GAMMA/4D0)*(F2*PE_N/(2D0*PE)-N0*N0*GAMMA/4D0)
*   *GAMMA)/(4D0*F2*PE_0))*ETA*ETA*ETA

C NUMERICAL INTEGRATION

  IFLAG=1
  XIN=ETA

```



```

      DETA=(.5D0-ETA)/DFLOAT(NPOINTS-1)
      XOUT=XIN+DETA
      NEQN=6
      F(1)=NN
      F(2)=NN_PR
      F(3)=FF
      F(4)=FF_PR
      F(5)=G0
      F(6)=GG_PR

      WRITE(9,100) z*0D0,N0/z
      WRITE(9,100) z*1D-2,NN/z
      WRITE(10,100) z*1D-2,FF_PR/ETA
      WRITE(11,100) z*0D0,0D0
      WRITE(11,100) z*1D-2,GG_PR
      WRITE(12,100) z*ETA,G0

      DO 5000 I=1,NPOINTS

      RELERR=RELERR0
      ABSERR=ABSERR0

1000  CALL RKf45(DERIVS,NEQN,F,XIN,XOUT,RELERR,ABSERR,IFLAG,WORK,IWORK)

      IF(IFLAG.EQ.2)GOTO 2002

      IF(IFLAG.EQ.3)THEN
      WRITE(6,200)
200  FORMAT("IFLAG=3: RELERR IS TOO SMALL")
      GOTO 1000
      ENDIF

      IF(IFLAG.EQ.4)THEN
      WRITE(6,201)
201  FORMAT("IFLAG=4: TOO MANY STEPS")
      GOTO 1000
      ENDIF

      IF(IFLAG.EQ.5)THEN
      WRITE(6,202)
202  FORMAT("IFLAG=5: ABSERR IS TOO SMALL")
      ABSERR=1D-10
      PAUSE
      GOTO 1000
      ENDIF

      IF(IFLAG.EQ.6)THEN
      WRITE(6,203)
203  FORMAT("IFLAG=6: REQUESTED ACCURACY IS TOO LARGE")
      RELERR=10D0*RELERR
      IFLAG=2
      GOTO 1000
      ENDIF

      IF(IFLAG.EQ.7)THEN
      WRITE(6,204)
204  FORMAT("IFLAG=7")

```

```

        IFLAG=2
        GOTO 1000
    ENDIF

    IF (IFLAG.EQ.8) THEN
        WRITE(6,205)
205    FORMAT("IFLAG=8: INVALID INPUT PARAMETERS")
        PAUSE
    ENDIF

2002    CONTINUE

        WRITE(9,100) z*XOUT,F(1)/z
        WRITE(10,100) z*XOUT,F(4)/XOUT
        WRITE(11,100) z*XOUT,F(6)
        WRITE(12,100) z*XOUT,F(5)
100    FORMAT(F20.10," ",F20.10)
        XOUT=XOUT+DETA

5000    CONTINUE

        CLOSE(9)
        CLOSE(10)
        CLOSE(11)
        CLOSE(12)

        STOP
        END

        SUBROUTINE DERIVS(ETA,F,DFDE)
            IMPLICIT REAL*8 (A-H)
            IMPLICIT REAL*8 (O-Z)
            DIMENSION F(6),DFDE(6)
            COMMON PE,PE_N,PE_0,GAMMA

C F(1)=N, F(2)=N', F(3)=F, F(4)=F', F(5)=G, F(6)=G'

            DFDE(3)=F(4)
            DFDE(4)=ETA*F(2)+F(4)/ETA
            DFDE(5)=F(6)
            DFDE(6)=- (1D0+PE_0*F(3))*F(6)/ETA+GAMMA*F(1)*F(1)
            DFDE(1)=F(2)
            DFDE(2)=- ( (1D0+F(3)*PE_N)/ETA-F(6)*PE)*F(2)
            * - (F(4)*PE_N/ETA-F(6)*PE/ETA-DFDE(6)*PE)*F(1)

            RETURN
            END

```