A FICK-JACOB’S EQUATION FOR CHANNELS OVER 3D CURVES

CARLOS VALERO VALDES
DEPARTAMENTO DE MATEMATICAS APLICADAS Y SISTEMAS
UNIVERSIDAD AUTONOMA METROPOLITANA-CUAJIMALPA
MÉXICO, D.F 01120, MÉXICO

RAFAEL HERRERA GUZMAN
CENTRO DE INVESTIGACIÓN EN MATEMÁTICAS (CIMAT)
GUANAJUATO, GTO
MÉXICO.

Abstract. The purpose of this paper is to provide a new formula for the effective diffusion coefficient of a generalized Fick-Jacob’s equation for narrow 3-dimensional channels. The generalized Fick-Jacob’s equation is obtained by projecting the 3-dimensional diffusion equation along the normal directions of a curve in three dimensional space that roughly resembles the narrow channel. The projection (or dimensional reduction) is achieved by integrating the diffusion equation along the cross sections of the channel contained in the planes orthogonal to the curve. We show that the resulting formula for the associated effective diffusion coefficient can be expressed in terms of the geometric moments of the channel’s cross sections and the curve’s curvature. We show the effect that a rotating cross section with offset has on the effective diffusion coefficient.

1. Introduction

Understanding spatially constrained diffusion in quasi-one dimensional systems is of fundamental importance in various sciences, such as biology (e.g. channels in biological systems), chemistry (e.g. pores in zeolites) and nano-technology (e.g. carbon nano-tubes). However, solving the diffusion equation in arbitrary channels is a very difficult task. One way to tackle it, which we follow in this paper, consists in reducing the degrees of freedom of the problem by considering only the main direction of transport.

The study of diffusion in (nearly) planar narrow channels has been undertaken and developed by several authors [3, 2, 5] following the approach of reducing the dimensionality of the problem to one dimension. They have provided formulas for estimates of the effective diffusion coefficient by "projecting" the two dimensional diffusion equation onto a straight line. More recently (see [8]), we have generalized this work by projecting the 2-dimensional diffusion onto an arbitrary curve on the plane, thus providing estimates of the effective diffusion coefficient involving the geometrical information of the curve (i.e. its curvature).

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In all the work mentioned above we can distinguish two cases: the infinite transversal diffusion rate case and the finite transversal diffusion rate case. In the former, it is assumed that the concentration distribution stabilizes instantly in the transversal directions of the channel and, in the latter, the finite time of transversal stabilization is taken into account. In mathematical terms this cases can be characterized as follows. In the first case the effective diffusion coefficient only involves 0-th order geometrical quantities of the channel (such as width). In the second case this coefficient involves higher order geometrical information, such as that arising from the tangential and curvature information (i.e. higher derivatives) of the channel’s surface wall(s).

On the other hand, the diffusion process in 3-dimensional (non-planar) channels presents more complications and remains a difficult problem to tackle. Some attempts have been carried out by Ogawa [6], Kalinay & Percus [5], Antipov et al [1]. Ogawa derived a formula for the effective diffusion coefficient for channels in 3-dimensional space over a central curve with constant rectangular cross section, and showed that the curvature of the central curve plays a fundamental role. Kalinay and Percus studied the case of a hyperboloidal cone. Antipov et al. studied the case of a periodically expanding and contracting straight channel.

The main motivation for using arbitrary curves in the dimensionality reduction technique is the following: by choosing a curve that "follows" the channel’s geometry as closely as possible, one is able to provide better estimates of the effective diffusion coefficient. If fact, we have shown in [8] that for two dimensional channels which are symmetric and of constant width, the formulas for the effective diffusion coefficient coincide in the finite and infinite transversal diffusion rate cases. In [6] Ogawa proved the same result for 3-dimensional having constant rectangular cross section.

Thus, the purpose of this paper is to derive a new formula for the effective diffusion coefficient (in the infinite transversal diffusion rate case) for 3-dimensional channels defined around a central curve in 3-dimensional space whose orthogonal cross section is not constant. We derive a formula for the effective diffusion coefficient with dependence on the curvature of the base curve, and the geometric and "statistical" properties of the cross section (i.e. its geometric moments). In particular, we derive explicit formulas relating the effective diffusion coefficient to the average rotation of the cross section of the channel with respect to the Frenet-Serret moving frame of the curve.

The outline of our article is as follows:

- In section 2, we will show how the three dimensional continuity equation on a channel can be reduced to a one dimensional continuity equation. This last equation, which we will call the effective continuity equation, will serve as the basis for what follows in the rest of the article.
- In section 3, we will derive a generalized Fick-Jacob’s equation and a new formula for the effective diffusion coefficient \( \mathcal{D} \) corresponding to the infinite transversal diffusion rate case (see formula (3.9)). The standard Fick-Jacob’s equation corresponds to the case when the base curve has zero curvature (i.e. it is a straight line). We will use standard tools of differential geometry of 3-dimensional curves to write down the formula for \( \mathcal{D} \).
A FICK-JACOB’S EQUATION FOR CHANNELS OVER 3D CURVES

2. THE EFFECTIVE CONTINUITY EQUATION ON A 3-DIMENSIONAL REGION

We are interested in describing a transport process on a channel-like region $\Omega$ in 3-dimensional space (see Figure 2.1).

The continuity equation. Let us assume that this process is modeled by the continuity equation

\[
\frac{\partial P}{\partial t} + \text{div}(J) = 0,
\]

where $P = P(x, y, z, t)$ is a real valued density function and $J = J(x, y, z, t)$ is the corresponding flux field. We will apply a dimensionality reduction technique to this equation as follows. Let $\Omega$ be parametrized by a smooth map $\varphi$ of the form

\[
\varphi(u, v, w) = (x(u, v, w), y(u, v, w), z(u, v, w)),
\]

where $u_1 \leq u \leq u_2$, $v_1 \leq v \leq v_2$ and $w_1 \leq w \leq w_2$. The parametrization $\varphi$ allows us to express $P$ and $J$ in terms of the $u, v, w$ coordinates by letting

\[
P(u, v, w, t) = P(x(u, v, w), y(u, v, w), z(u, v, w), t),
\]

\[
J(u, v, w, t) = J(x(u, v, w), y(u, v, w), z(u, v, w), t).
\]

For each $u$ we will let $\Omega_u$ be the sub-region of $\Omega$ consisting of the points of the form $\varphi(s, v, w)$ such that $u_1 \leq s \leq u$, and $S_u$ be the cross section parametrized by the map $(v, w) \mapsto \varphi(u, v, w)$ (see Figure 2.1).

Dimensional reduction of the continuity equation. From calculus in several variables, the total concentration of $P$ in $\Omega_u$ is given by

\[
C(u, t) = \int_{u_1}^{u} \left( \int_{w_1}^{w_2} \int_{v_1}^{v_2} P(s, v, w, t) \det(\varphi'(s, v, w)) dv dw \right) ds,
\]

Figure 2.1. Region $\Omega_u$ and cross section $S_u$

- In section 4 we study channels with gyrating cross section and deduce Ogawa’s formula [6] as a particular case.
- We finish with conclusions in section 5 and a brief review of the necessary differential geometric material in the Appendix.
where $\phi'$ is the Jacobian matrix of $\phi$. The effective density $p$ is defined as

$$p(u, t) = \frac{dC}{du}(u, t) = \int_{w_1}^{w_2} \int_{v_1}^{v_2} P(u, v, w, t) \det(\phi'(u, v, w)) dvdw,$$

and the effective flux $j$ by

$$j(u, t) = \int_{w_1}^{w_2} \int_{v_1}^{v_2} J(u, v, w, t) \cdot \left( \frac{\partial \phi}{\partial v}(u, v, w) \times \frac{\partial \phi}{\partial w}(u, v, w) \right) dvdw,$$

where we have denoted the dot product by $\cdot$ and the cross product by $\times$. The quantity $p(u, t)$ measures the concentration density at time $t$ along the cross section $S_u$, and $j(u, t)$ measures the flux density along $S_u$. Let $\partial \Omega$ denote the border of the region $\Omega$ and assume that there is no flux of $P$ across $\partial \Omega \setminus (S_{u_1} \cup S_{u_2})$. Then by using the continuity equation (2.1) and the divergence theorem we obtain the effective continuity equation

$$\frac{\partial p}{\partial t}(u, t) + \frac{\partial j}{\partial u}(u, t) = 0.\quad (2.2)$$

**Diffusion equation.** By imposing Fick's law

$$J = -D \nabla P,$$

for a constant diffusion coefficient $D$ and where $\nabla P$ denotes the gradient of $P$ in the spatial directions, the continuity equation (2.1) becomes the diffusion equation

$$\frac{\partial P}{\partial t} = D \Delta P,$$

where $\Delta$ is the laplacian operator given by

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

In this case, the 1-dimensional effective flux becomes

$$j(u, t) = -D \int_{w_1}^{w_2} \int_{v_1}^{v_2} \nabla P(u, v, w, t) \cdot \left( \frac{\partial \phi}{\partial v}(u, v, w) \times \frac{\partial \phi}{\partial w}(u, v, w) \right) dvdw,$$

where

$$\nabla P(u, v, w, t) = \left( \frac{\partial P}{\partial x}(\phi(u, v, w), t), \frac{\partial P}{\partial y}(\phi(u, v, w), t), \frac{\partial P}{\partial z}(\phi(u, v, w), t) \right).$$

3. **A generalized Fick-Jacob’s equation on the normal bundle of a 3-dimensional curve: infinite transversal diffusion rate case**

In this section we derive a generalized Fick-Jacob’s equation and a new formula for the effective diffusion coefficient (corresponding to the infinite transversal diffusion rate) for channels that "follow" a base curve in 3-dimensional space.
Channel set-up. Let $\alpha = \alpha(u)$ be a curve in three dimensional space parametrized by the arc-length parameter $u$, and consider scalar functions $\eta = \eta(u, v, w), \beta = \beta(u, v, w)$. Let $\Omega$ be the channel-like region parametrized by the map

$$\varphi(v, w) = \alpha(u) + \eta(u, v, w)N(u) + \beta(u, v, w)B(u),$$

where $N$ and $B$ are the normal and binormal fields of $\alpha$ (see Appendix). In this case, each cross section $S_u$ is contained in the plane passing through $\alpha(u)$ and spanned by the vectors $N(u)$ and $B(u)$. By having arbitrary smooth functions $\beta$ and $\eta$ as coefficients we can generate very general cross sections $S_u$. Using the Frenet-Serret formulae we obtain

$$\frac{d\varphi}{du} = (1 - \eta\kappa) T + \left( \frac{\partial \eta}{\partial u} - \beta\tau \right) N + \left( \frac{\partial \beta}{\partial u} + \eta\tau \right) B,$$

$$\frac{\partial \varphi}{\partial v} = \frac{\partial \eta}{\partial v} N + \frac{\partial \beta}{\partial v} B,$$

$$\frac{\partial \varphi}{\partial w} = \frac{\partial \eta}{\partial w} N + \frac{\partial \beta}{\partial w} B,$$

where $\kappa$ and $\tau$ are the curvature and torsion functions associated to $\alpha$. From these formulas we deduce that

$$\text{det}(\varphi') = \omega_S(1 - \eta\kappa),$$

$$\frac{\partial \varphi}{\partial v} \times \frac{\partial \varphi}{\partial w} = \omega_S T,$$

where

$$\omega_S = \text{det} \left( \begin{array}{ccc} \frac{\partial \eta}{\partial v} & \frac{\partial \eta}{\partial w} \\ \frac{\partial \beta}{\partial v} & \frac{\partial \beta}{\partial w} \end{array} \right).$$

The map $(v, w) \mapsto \omega_S(u, v, w)$ is the area density function of the cross section $S_u$, so that

$$A(u) = \int_{u_1}^{u_2} \int_{v_1}^{v_2} \omega_S(u, v, w) dv dw,$$

is the area of $S_u$. Given a function $f = f(v, w)$, its integral on $S_u$ is given by

$$\int_{S_u} f = \int_{u_1}^{u_2} \int_{v_1}^{v_2} f(v, w) \omega_S(u, v, w) dv dw,$$

i.e. we integrate $f$ over $S_u$ by using the area element $\omega_S(u, v, w) dv dw$. The average value of $f$ over $S_u$ is then expressed as

$$(f)_u = \frac{1}{A(u)} \int_{S_u} f.$$

In order to simplify notation, we will write $(f)$ for the function $u \mapsto (f)_u$.

Infinite transversal diffusion rate. The assumption of infinite transversal diffusion rate means that $P$ is independent of the variables $v$ and $w$. In this case, we have that the effective density (2.2) is given by

$$p(u, t) = \omega(u) P(u, t)$$

where

$$\omega(u) = \int_{v_1}^{v_2} \int_{u_1}^{u_2} \text{det}(\varphi'(u)) dv dw.$$

The function $\omega(u)$ is the volume density function with respect to $u$, so that

$$V(u) = \int_{u_0}^{u} \omega(s) ds.$$
is the volume of the region $\Omega_u$. By using formula (3.2) we obtain

$$\omega(u) = \int_{S_u} (1 - \kappa \eta) = A(u)(1 - \kappa(u)\langle\eta\rangle_u).$$

To compute the effective flux (2.3) observe that $P$ is constant along the planes passing through $\alpha(u)$ and spanned by $N(u)$ and $B(u)$. Hence $\nabla P$ is orthogonal to $N$ and $B$ so that

$$\frac{\partial P}{\partial u} = \nabla P \cdot \frac{\partial \varphi}{\partial u} = (1 - \eta \kappa) \nabla P \cdot T,$$

where $\nabla P$ is the gradient of $P$ with respect to the $x, y, z$ variables. Using this and formulas (2.3) and (3.3), we obtain

$$j(u, t) = -D \frac{\partial P}{\partial u}(u, t) \int_{S_u} (1 - \eta \kappa)^{-1}.$$

By using equation (3.4) and letting

$$D(u) = D \left( \frac{\int_{S_u} (1 - \eta \kappa)^{-1}}{\int_{S_u} (1 - \eta \kappa)} \right)$$

$$= D \left( \frac{\langle(1 - \eta \kappa)^{-1}\rangle_u}{1 - \kappa \langle\eta\rangle_u} \right),$$

formula (3.5) for $j$ can be written as

$$j(u, t) = -D(u)\omega(u) \frac{\partial}{\partial u} \left( \frac{p(u)}{\omega(u)} \right).$$

**Generalized Fick-Jacob’s equation and effective diffusion coefficient.** If we substitute formula (3.7) into the effective continuity equation (2.2) we obtain the following generalized Fick-Jacob’s equation

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial u} \left( D(u)\omega(u) \frac{\partial}{\partial u} \left( \frac{p(u, t)}{\omega(u)} \right) \right),$$

which, in turn, casts

$$D(u) = D \left( \frac{\langle(1 - \eta \kappa)^{-1}\rangle_u}{1 - \kappa \langle\eta\rangle_u} \right).$$

as the effective diffusion coefficient.

**Remark.** When $\kappa = 0$, we have that $D \equiv D$ and $\omega(u) = A(u)$, and the above generalized Fick-Jacks becomes the classical Fick-Jacks equation

$$\frac{\partial p}{\partial t} = D \frac{\partial}{\partial u} \left( A(u) \frac{\partial}{\partial u} \left( \frac{p(u, t)}{A(u)} \right) \right).$$
Central curve. From the definition of $\varphi$ we have that
\[ \langle \varphi \rangle_u = \alpha(u) + \eta N(u) + \beta B(u). \]
Hence, $\langle \eta \rangle_u$ is the $N(u)$ component of $\langle \varphi \rangle_u$ when taking $\alpha(u)$ as reference point. We will refer to the curve $\langle \varphi \rangle$ as the central curve of the channel defined by $\varphi$.

*Remark.* Since the volume of the region $\Omega_u$ is given by
\[ V(u) = \int_{u_1}^u A(u)(1 - \kappa(u)\langle \eta \rangle_u)du, \]
when $\alpha$ and $\langle \varphi \rangle$ coincide, we have $\langle \eta \rangle \equiv 0$ and
\[ V(u) = \int_{u_1}^u A(u)du. \]
For $\alpha$ a circle, the last formula is the well known Pappus theorem which establishes how to compute the volumes of solids of revolution.

**Geometric moments.** We can get a better understanding of the function $\langle (1 - \eta \kappa)^{-1} \rangle$ appearing in the numerator of $\mathcal{D}$, by considering the geometric series expansion
\[ (1 - \eta \kappa)^{-1} = \sum_{n=0}^{\infty} \eta^n \kappa^n. \]
Observe that the lower order terms in this series dominate when $\kappa \eta < 1$, i.e. when the $\eta$ coordinates of the channel are far away from the focal points $\alpha + N/\kappa$ of the base curve $\alpha$. This last condition is consistent with our narrow channel assumption. Using the above expansion we can write
\[ \langle (1 - \eta \kappa)^{-1} \rangle = \left( \sum_{i=0}^{\infty} \langle \eta^i \rangle \kappa^i \right), \]
We will refer to the functions $\langle \eta^i \rangle$ as the channel’s $\eta$–moments. Hence, we can write
\[ \mathcal{D}(u) = \left( \frac{D}{1 - \kappa(u)\langle \eta \rangle} \right) \sum_{i=0}^{\infty} \langle \eta^i \rangle \kappa^i. \]

*Remark.* Observe that when $\kappa = 0$, we have $\mathcal{D}(u) = D$, and hence all the geometric information provided by the $\eta$ moments of the channel is lost. This is, in fact, a good reason why to study the projection of diffusion along general (non-straight) curves.

**The first three geometric moments.** We will now use the first three terms in the series (3.10) to relate the effective diffusion coefficient $\mathcal{D}$ to geometric properties of the channel. Consider the symmetric matrix
\[ M(u) = \begin{pmatrix} a(u) & c(u) \\ c(u) & b(u) \end{pmatrix}, \]
where
\[ a = \langle (\eta - \langle \eta \rangle)^2 \rangle, \]
\[ b = \langle (\beta - \langle \beta \rangle)^2 \rangle, \]
\[ c = \langle (\eta - \langle \eta \rangle)(\beta - \langle \beta \rangle) \rangle. \]
The eigenvectors and eigenvalues of \( M(u) \) can be used to measure the average orientation angle \( \theta(u) \) and average sizes \( s_1(u) \) and \( s_2(u) \) of the cross section \( S_u \) in the \( N(u) \) and \( B(u) \) directions with respect to its central point \( \langle \varphi \rangle_u \) (see Figure 3.1). Let \( \lambda_1(u) \) and \( \lambda_2(u) \) be the ordered eigenvalues of \( M(u) \) such that \( \lambda_1(u) \geq \lambda_2(u) \). The angle \( \theta(u) \) is the one formed between \( N(u) \) and the eigenvector of \( M(u) \) corresponding to \( \lambda_1(u) \), and the functions \( s_1 \) and \( s_2 \) are given by the formulas

\[
\begin{align*}
    s_1(u) &= 2\sqrt{\lambda_1(u)} \\
    s_2(u) &= 2\sqrt{\lambda_2(u)}.
\end{align*}
\]

Some simple algebra then shows that

\[
\begin{align*}
    a &= \left( \frac{s_1}{2} \right)^2 \cos^2(\theta) + \left( \frac{s_2}{2} \right)^2 \sin^2(\theta), \\
    b &= \left( \frac{s_2}{2} \right)^2 \cos^2(\theta) + \left( \frac{s_1}{2} \right)^2 \sin^2(\theta), \\
    c &= \left( \frac{s_1}{2} \right)^2 - \left( \frac{s_2}{2} \right)^2 \cos(\theta)\sin(\theta).
\end{align*}
\]

Hence

\[
\langle \eta^2 \rangle = \langle \eta \rangle^2 + \left( \frac{s_1}{2} \right)^2 \cos^2(\theta) + \left( \frac{s_2}{2} \right)^2 \sin^2(\theta).
\]

Using the above formulas and the first three terms of the series (3.10) we obtain the following approximation

\[
D \approx \frac{D(1 + \langle \eta \rangle \kappa + \left( \frac{s_1}{2} \right)^2 \cos^2(\theta) + \left( \frac{s_2}{2} \right)^2 \sin^2(\theta) \kappa^2)}{(1 - \kappa \langle \eta \rangle)}.
\]

**Higher order moments.** The higher order moments of \( \eta \), i.e. the functions \( \langle \eta^i \rangle \) for \( i > 2 \), contain more subtle information of the geometry of the channel than that provided by the moments of order 0, 1 and 2. For example, in the context of probability distributions concepts like skewness and kurtosis, which are a measure the asymmetry and "peakedness" of a distribution (respectively) involve in their
A FICK-JACOB’S EQUATION FOR CHANNELS OVER 3D CURVES

4. Applications - Twisted channels with offsets

In this section we will apply our results to show how our formula for the effective diffusion coefficient captures information about the way the cross section of a channel gyrates with respect to the Frenet-Serret frame, as well as the effects of offsets from the base curve. We deduce Ogawa’s formula \[ \text{[6]} \] as a particular case.

We will consider a parametrisation \( \varphi \) of the form \([4.1]\) where \( \eta \) and \( \beta \) are constructed as follows. For a fixed planar region \( R_0 \) parametrized by the the map \((4.1)\)

\[
(\eta_0, \beta_0) \rightarrow (\eta_0(v, w), \beta_0(v, w)),
\]

we let \( \eta, \beta \) be given by

\[
\begin{pmatrix}
\eta(u, v, w) \\
\beta(u, v, w)
\end{pmatrix}
= \begin{pmatrix}
\cos(\omega u) & -\sin(\omega u) \\
\sin(\omega u) & \cos(\omega u)
\end{pmatrix}
\begin{pmatrix}
\eta_0(v, w) \\
\beta_0(v, w)
\end{pmatrix}
+ \begin{pmatrix}
p(u) \\
q(u)
\end{pmatrix}
\]

For a given curve \( \alpha \), the above \( \varphi \), with the above \( \eta \) and \( \beta \), represents a channel constructed by rotating region \( R_0 \) with angular velocity \( \omega \) (as we move along the \( u \)-variable) with respect to the Serret-Frenet frame of \( \alpha \), and having offset \( p(u)N(u) + q(u)B(u) \) from \( \alpha(u) \).

4.1. Twisted elliptical cross sections with offsets. A solid ellipse with mayor and minor radii \( r_1 \) and \( r_2 \), where \( r_1 > r_2 \), can be parametrised by the map \([4.1]\) with

\[
\eta_0 = vr_1 \cos(w) \quad \text{and} \quad \beta_0 = vr_2 \sin(w),
\]
for $0 \leq v \leq 1$ and $0 \leq w \leq 2\pi$. If use $\eta$ and $\beta$ defined by formula (1.2), then the average sizes and the area of the channel’s cross sections are given by

$$s_1 = r_1, s_2 = r_2 \quad \text{and} \quad A = \pi r_1 r_2,$$

and the effective diffusion coefficient by (see Figure 4.1)

$$D(u) = \frac{2}{\kappa^2(u)(r_1^2 \cos^2(\omega u) + r_2^2 \sin^2(\omega u))}.$$

If there is no gyration, i.e. $\omega = 0$, the above formula becomes

$$D(u) = \frac{2}{\kappa^2(u)r_1^2}.$$

It is interesting to observe that in this case the offset functions $p$ and $q$ do no enter into the above formulas.

4.2. Twisted rectangular cross sections with offsets. A solid rectangle with sides $d_1$ and $d_2$ can be parametrised by map (1.1) by letting

$$\eta_0 = v \quad \text{and} \quad \beta_0 = w,$$

for $-d_1/2 \leq v \leq d_1/2$ and $-d_2/2 \leq w \leq d_2/2$. We then have

$$s_1 = d_1/\sqrt{3}, s_2 = d_2/\sqrt{3} \quad \text{and} \quad A = d_1 d_2$$

In this case we obtain

$$D(u) = \frac{\sum_{i=1}^4 (-1)^{i+1} \gamma_i(u) \log(\gamma_i(u))}{d_1 d_2 (1 - \kappa(u)p(u)) \kappa^2(u) \cos(\omega u) \sin(\omega u)},$$

where

$$\gamma_i(u) = 1 - \kappa(u)(p(u) + (\cos(\omega u), \sin(\omega u)) \cdot z_i)$$

and

$$z_1 = \frac{1}{2}(d_1, d_2), z_2 = \frac{1}{2}(d_1, -d_2), z_3 = \frac{1}{2}(-d_1, d_2) \quad \text{and} \quad z_4 = \frac{1}{2}(-d_1, -d_2).$$

When there is no gyration we have that

$$D(u) = \frac{1}{\kappa(u)d_1} \log \left( \frac{1 + \kappa(u)(d_1/2 - p(u))}{1 - \kappa(u)(d_1/2 + p(u))} \right).$$

For $p = 0$, the above formula is the one obtained by Ogawa in [6]. Observe that, in contrast to the formulas of the previous subsection, in this case the offset function $p$ does enter into the formulas for the effective diffusion coefficient $D$.

4.3. Twisted cardioidal cross sections with offsets. In this case we have that

$$\eta_0 = vr(2 \cos(w) - \cos(2w)) \quad \text{and} \quad \beta_0 = vr(2 \sin(w) - \sin(2w)),$$

where the parameter $r$ is the radius of the circle used to construct the cardioidal curve. The interior of the region shown in the left part of Figure 4.3 is the region parametrised by the map $(v, w) \mapsto (\eta_0(v, w), \beta_0(v, w))$ for $0 \leq v \leq 1$ and $0 \leq w \leq 2\pi$. The right part of the figure shows the channel resulting from gyrating this cross section over the Frenet-Serret frame of a helix. The parameters of the helix are $a = 1, b = 1/4$ and the gyration velocity is $\omega = 2$. Under the above hypotheses we obtain

$$s_1 = \sqrt{7}r, s_2 = \frac{\sqrt{17}}{3}r \quad \text{and} \quad A = 6\pi r^2.$$

A FICK-JACOB’S EQUATION FOR CHANNELS OVER 3D CURVES 10
In contrast with the previous two cases, the mean curve $<\varphi>_u$ does not coincide with the base curve $\alpha$ and, in fact, we have that

$$<\varphi>_u = \alpha(u) + \left(p - \frac{2}{3}r\cos(\omega u)\right)N(u) + \left(q - \frac{2}{3}r\sin(\omega u)\right)B(u).$$

Computing the integrals that define the effective diffusion coefficient we obtain

$$D(u) = \frac{2(1 - p(u)\kappa(u))}{r^2\kappa^2(u)(3 - 3p(u)\kappa(u) + 2r\kappa(u)\cos(\omega u)).}$$

If we let

$$p(u) = \frac{2}{3}r\cos(\omega u) \quad \text{and} \quad q(u) = \frac{2}{3}r\sin(\omega u),$$

then the mean curve $<\varphi>$ coincides with $\alpha$, and in this case we obtain that

$$D(u) = \frac{6 - 4r\kappa(u)\cos(\omega u)}{9r^2\kappa^2(u)}.$$

### 4.4. Comparing the elliptical and cardioid cases

We conclude by comparing the elliptical and cardioid effective diffusion formulas given in the previous subsections. To do a "fair" comparison we need to set the parameters of the cross sections so that their geometries are as similar as possible. We do this by equating their geometric moments up to order 2, i.e. the mean curves, the width functions $s_1$ and $s_2$, and the orientation function $\theta$ must coincide for both channels. Since the mean curve in the elliptical case coincides with the curve $\alpha$, we must use the offsets (4.4).

Equating the width functions in both cases implies that the major and minor radii of the elliptical cross section must satisfy

$$r_1 = \sqrt{7}r \quad \text{and} \quad r_2 = \frac{\sqrt{47}}{3}r.$$

For the angle functions $\theta$ to be equal we simply use the same $\omega$ as the gyrating velocity in both cases. Using this assumptions and letting $D_e$ and $D_c$ stand of the effective diffusion coefficient in the elliptical and cardioid case, respectively, we obtain

$$D_c(u) = \frac{6 - 4r\kappa^2(u)\cos(\omega u)}{9r^2\kappa^2(u)}.$$
and

\[ D_e(u) = \frac{2}{\kappa^2(u)(7r^2 \cos^2(\omega u) + (47/9)r^2 \sin^2(\omega u))} \]

In the left part of Figure 4.4 we show the cross sections of the elliptical and cardioidal channels with the parameters described above. The right part of the figure shows the corresponding effective diffusion coefficients, where the base curve \( \alpha \) is an helix with parameters \( a = 1, b = 1/4 \), the parameter of the cardioid is \( r = 1/6 \) and the gyration velocity is \( \omega = 1 \).

5. Conclusions and future work

We have deduced a new formula for the effective diffusion coefficient \( D \) of a generalized Fick-Jacobs equation for narrow 3-dimensional channels. We derived such an formula by projecting the diffusion equation along the normal directions of a base curve of a narrow channel in 3-dimensional space under the assumption of infinite transversal diffusion rate, and using tools of differential geometry of curves. Our formula establishes an explicit relation between some of the channel’s geometric properties (i.e. curvature of the base curve and the geometric moments of the transversal cross sections) and the corresponding effective diffusion coefficient. We have also showed that previous estimates [6] for \( D \) can be recovered from our formula as particular cases, and how our formula captures information about the way the cross sections gyrate with respect to the Frenet-Serret frame.

In future work, we will deal with the case of finite transversal diffusion rate case. We expect that in that case both tangential and curvature information of the channel’s surface will enter into the formula of the effective diffusion coefficient.

6. Appendix - The Serret-Frenet formulas for 3D curves.

In this appendix we review some basic concepts of the differential geometry of curves in three dimensional space. The material is standard and can be found in books such as [7, 4]. Consider a smooth curve in three dimensional space of the form \( \alpha(s) = (x(s), y(s), z(s)) \). The curve is said to have arc-length parametrization
if for all $s$ in the interval $[s_1, s_2]$ we have that
\[ \left| \frac{d\alpha}{ds} \right| = 1 \quad \text{where} \quad \left| \frac{d\alpha}{ds} \right| = \sqrt{\left( \frac{dx}{ds} \right)^2 + \left( \frac{dy}{ds} \right)^2 + \left( \frac{dz}{ds} \right)^2}. \]

If the above condition holds, then the length of the curve segment $\alpha([s_1, s])$ is given by
\[ \text{length}(\alpha([s_1, s]) = \int_{s_1}^{s} \left| \frac{d\alpha}{ds} (a) \right| da = s. \]

We can construct three orthonormal fields to $\alpha$ given by
\[ T = \frac{d\alpha}{ds}, \quad N = \frac{dT}{ds} / \left| \frac{dT}{ds} \right| \quad \text{and} \quad B = T \times N, \]
which are known as the tangent, normal and bi-normal fields, respectively. The orthonormality conditions on these fields imply the existence of scalar functions $\kappa = \kappa(u)$ and $\tau = \tau(u)$, known as the curvature and torsion, such that
\[ \frac{dT}{ds} = \kappa N, \]
\[ \frac{dN}{ds} = -\kappa T + \tau B, \]
\[ \frac{dB}{ds} = -\tau N. \]

These formulas are known in the literature as the Frenet-Serret formulas, and the fields $T, N, B$ as the Frenet-Serret frame. The curvature function measures the deviation of $\alpha$ of being a straight line, and $\tau$ the deviation of $\alpha$ from being in a plane.

As an example, consider a helix of radius $a > 0$ and pitch $b > 0$ parametrised by
\[ s \mapsto (a \cos(s), a \sin(s), bs). \]

The arc-length parametrisation of this curve is
\[ \alpha(u) = (a \cos(\sqrt{1-b^2u}/a), a \sin(\sqrt{1-b^2u}/a), bu), \]
and the corresponding curvature and torsion of this curve are
\[ \kappa = \frac{a}{a^2 + b^2} \quad \text{and} \quad \tau = \frac{b}{a^2 + b^2}. \]

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