SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: **TD1409**
STSM title: **Solution Landscapes in Nematic Microfluidics**
STSM start and end date: **08/05/2017** to **19/05/2017**
Grantee name: **María Crespo Moya**

PURPOSE OF THE STSM:

My scientific collaboration with the Complex Fluids Research Group, led by Dr Ian Griffiths (Senior Research Fellow at the University of Oxford), started on April 2014, when I participated both in the OCCAM 6th UK Graduate Modelling Camp and the 100th European Study Group with Industry. At the Mathematical Institute, Ian Griffiths introduced me to Dr Apala Majumdar (OCIAM Visiting Fellow from University of Bath). The three of us identified a problem in the field of Nematic Microfluidics that required the unification of all of our skills. Our collaboration continued through two academic stays at the Mathematical Institute, funded by the Spanish Government, with a total duration of 5 months during the summers of 2015 and 2016. Additionally, Ian Griffiths was one of the external reviewers of my thesis work, while Apala Majumdar was member of the tribunal in my thesis defense.

This STSM represented the ideal framework to reinforce my skills in the application of mathematics to nematic microfluidics and to establish a new network between the scientific and academic Oxford community, the applied and interdisciplinary mathematics group at Bath and my new research base in the MODEMIC research group in Montpellier.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

During my STSM, I have been working in collaboration with professors Apala Majumdar, Ian Griffiths, Dirk Aarts and Louis Cortes, visiting both the University of Oxford and the University of Bath. Through this collaboration, we tackled two different problems:

Liquid Crystals:
Liquid crystals are states of matter which are sometimes observed to occur between the solid crystal state and the conventional liquid state. In the simplest description, liquid crystals can be thought of as elongated rod-like molecules which have a preferred local average direction. Here, we focus on two different phases of liquid crystals: *nematic phase* (molecules possess directional order but no positional order, i.e., they are randomly distributed as in a liquid) and *smectic phase* (molecules show directional order and positional order, i.e., they are arranged in some ordered pattern).
Experimentalists use a suspension of nano-inclusions or silica particles in an isotropic fluid and observe structural transitions as a function of the concentration of the nano-inclusions. Within a rectangular chamber,

they observe disordered profiles at the top, orientationally ordered nematic profiles at intermediate heights and orientationally and layered smectic-like profiles at the cell bottom.
We aim to mimic the experimental profiles by using a liquid crystal model that can account for smectic, nematic and isotropic phases.

Bioreactors:
A bioreactor is a vessel in which a biological reaction occurs between two substances: a substrate (e.g. nitrite) and a microorganism (e.g. bacteria), which develops by substrate consumption. During my PhD, I proposed a coupled system of Advection-Diffusion-Reaction equations, together with boundary conditions of mixed type, in order to describe the dynamics in the continuous bioreactor.
There exists an static equilibrium of this system, usually called *washout*, in which the bacteria becomes extinct and the substrate concentration remains constant. By numerically computing the solution of this PDE system, one may observe that, under suitable conditions, another asymptotically steady state (different from the washout) exists.
In [1], the authors considered the one-dimensional version of the bioreactor model and, assuming that both biomass and substrate diffuse through the water in the vessel with the same diffusion rate, they mathematically prove the existence of a second steady state.

[1] A.K. Dramé, C. Lobry, J. Harmand, A. Rapaport, and F. Mazenc. Multiple stable equilibrium profiles in tubular bioreactors. *Mathematical and Computer Modelling*, 48(11):1840 – 1853, 2008.

This state can be seen as the solution of a nonlinear second order ordinary differential equation, the solution of which is not written explicitly but approximated numerically. We aim to study the multiplicity of steady states of the model and characterize the non-constant equilibrium solutions.

Additionally, my stay in the UK gave me the opportunity to give two seminars:

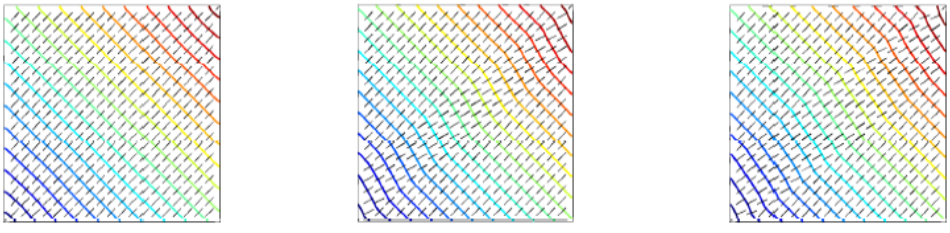
- 10th May: *Optimal shape of a continuous bioreactor used for water treatment processes*. Complexity Cluster Workshop, Advanced Studies Centre of the Keble College (University of Oxford).
- 15th May: Solution Landscapes in Nematic Microfluidics. Nonlinear Mechanics Seminar, Department of Mathematical Sciences of the University of Bath.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The main outcomes have been:

Liquid Crystals:

- Formulation of a first mathematical model that describes the layer profiles and the average director of molecular alignment. This model consists in a coupled system of elliptic equations, completed with Dirichlet and Neumman boundary conditions.
- Numerical simulation of the model solution by using the software COMSOL Multiphysics. We conclude that different molecular orientation is observed depending on the model parameters. Some examples can be observed in Figure 1, which seem to show that the molecules are arranged in layers, the layer profile changing with model parameters. Nevertheless, the nature of the obtained layer forms does not fully agree with the experimental observations.



(a) Alignment Type 1 (b) Alignment Type 2 (c) Alignment Type 3

Figure 1: Schematic representation of the possible molecular alignments depending on the model parameters. The black represent the molecules, while the colored lines represent the layer profiles among which the molecules are arranged.

- Formulation of a second mathematical model based on Landau-de Gennes theory, where the resulting layer profile and the molecular alignment can be seen as minimizers of the Landau-de Gennes free energy (see, e.g., [2],[3]). This model consists in a coupled system of elliptic equations, much more complex than the one proposed at a first stage, completed with Dirichlet and Neumman boundary conditions.

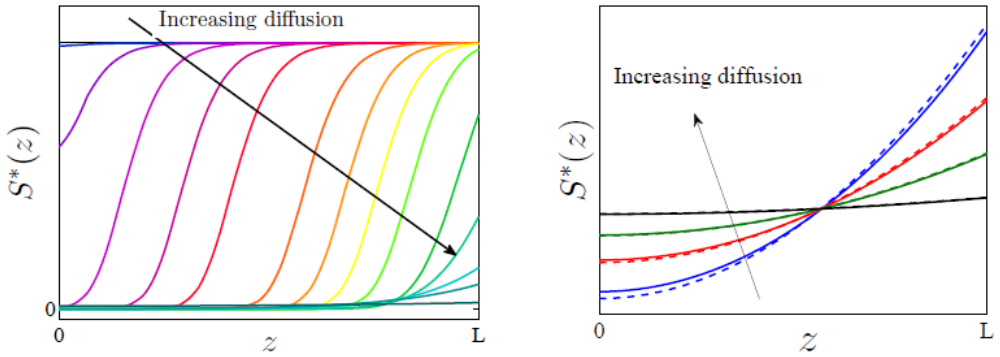
[2] C. Luo, A. Majumdar, and R. Erban. Multistability in planar liquid crystal wells. *Physical Review E*, 85(061702), 2012.

[3] M. Robinson, C. Luo, P.E. Farrell, R. Erban, and A. Majumdar. From molecular to continuum modelling of bistable liquid crystal devices. *Liquid Crystals*, 2017.

- Numerical simulation of the model solution by using the software COMSOL Multiphysics. Tentative first steps were made in this area during the academic stay.

Bioreactors:

- Postulating a methodology to analytically tackle the problem of existence of the second steady state when dropping the assumption that both biomass and substrate show the same diffusion rate. We aim to interpret the governing equations as Euler-Lagrange equations of an appropriately defined functional and use variational methods to prove that the energy associated to the system has a non-constant minimizer, which corresponds to the second steady state.
- Applying asymptotic analysis in order to approximate the second steady state in the cases where the diffusion coefficients of the species are either really small or really large compared with the rest of model parameters. This work has allowed us to obtain a explicit expression of the second steady state. Figure 2 shows the comparison between the steady state obtained either by numerical simulation of the full bioreactor model or using asymptotic analysis.



(a) Steady states (approximated numerically) for different diffusion coefficients

(b) Comparison of asymptotic solution (dashed) with the full numerical solution to (solid) for large diffusion coefficients.

Figure 2: Graphical interpretation of the substrate concentration at steady state, denoted by $S^*(z)$, as a function of the reactor height, $z \in [0, L]$.

FUTURE COLLABORATIONS (if applicable)

The collaboration carried out during this Short Term Scientific Mission was a first step towards modelling two interesting mathematical problems, which solution are non-trivial and may have a strong impact from the experimentalist point of view. We aim to continue this collaboration by keeping in touch by e-mail and regular Skype meetings. Once the expected results are obtained, these two works will be sent to scientific journals with high international impact.