Software development and numerical simulation of the heterogeneity in transport diffusion with nutrients and micro-organisms

Presentation of the subject

The framework of the subject is to consider a general model of networks of interconnected o.d.e. that represents heterogeneity in transport diffusion:

1. either of inert chemicals,
2. either of reactive chemicals with biomass ,
3. or both

based on two formalisms developed in the literature:

− the linear input/output models of MINC/MRMT kinds (ref [3]) for case 1,
− the general (nonlinear) gradostat models (ref [5]) for case 2.

The targeted applications are

− Propagation of pollutants in water resources such as lakes or water tables (case 1).
− Microbial degradation of pollutants in soils with a focus on biogas outputs (case 2).
− Landfill exploitations (case 3).

These researches are part of current collaborations with Chile (Inria Associated Team DYMECOS and REDES project) and the recently accepted French ANR project MicroSoil3D.

Objectives of the internship

The expected work is twofold:

1. Conceive and write in Python (with numpy and matplotlib modules) a simulator of such networks of o.d.e. proposing convivial ways of parameters choices and outputs representations, and that could be a support for future modules extensions
2. Develop two first modules: one to compute equivalent input/output networks for case 1 and a second one to identify reduced structures from larger ones, based on the mathematical theory of input/output systems.

Depending on the profile and motivations of the candidate, emphasis could be made on the user interface, the algorithms or the applications. This work could lead to a continuation in forthcoming internships about developing extensions related to optimization:

− static optimization of networks for a given output (optimal design for the biotechnology industry)

optimal control of the inputs for the minimal time to achieve a target (ex. decontamination) or the integral cost on a given time interval (ex. biogas production)

Candidate profile

The expected skills of the candidate are a good knowledge of the theory differential equations (ref. [4] for instance) and numerical analysis (ref [2] for instance), and a taste for programming. Knowledge on automatic control (ref [1] for instance) would be an added value, although not compulsory.

Organization of the internship

The candidate will be incorporated in the Modemic team at the Mistea Lab, Campus Inra/SupAgro, Montpellier under the supervision of A. Rapaport, and will have opportunities to exchange with other researchers and PhD students on related subjects. Duration, dates and salary can be discussed.

References

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[4] L. Perko. Differential equations and dynamical systems. 3rd ed. Springer, 2001.

[5] H. Smith, P. Waltman. The theory of the chemostat, dynamics of microbial competition. Cambridge University Press, 1995.

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