Comput. Methods Appl. Mech. Engrg. 272 (2014) 271–289

Contents lists available at ScienceDirect

Comput. Methods Appl. Mech. Engrg.

journal homepage: www.elsevier.com/locate/cma

A new approach to the simulation of microbial biofilms by a theory of fluid-like pressure-restricted finite growth

Antonio Bolea Albero [a], Alexander E. Ehret [b], Markus Böl [a,*]

[a] Institute of Solid Mechanics, Technische Universität Braunschweig, 38106 Braunschweig, Germany
[b] Institute of Mechanical Systems, ETH Zurich, 8092 Zurich, Switzerland

ARTICLE INFO

Article history:
Received 29 September 2013
Received in revised form 5 December 2013
Accepted 1 January 2014
Available online 23 January 2014

Keywords:
Continuum mechanics
Biofilm growth
Pressure restriction
Finite viscoelasticity

ABSTRACT

In general, the term 'growth' characterises the process by which a living body increases in size by addition of mass. Living matter grows in various different ways, triggered by genetic and biological factors. In addition, the configuration of the grown body in space depends on its interaction with the environment at the boundaries. In this paper, we deal with mechanical constraints on growth at the boundary of the body. Particularly, we present a model for growth such that residual stresses resulting from an isotropic deposition of new material are continuously relieved and that depends on the hydrostatic pressure acting on the material. As an example for this pressure-restricted fluid-like type of growth, we consider microbial biofilms growing between rigid obstacles in geometrically confined environments. The presented concept unites two classical constitutive formulations of large strain viscoelasticity and finite growth. The model was implemented into a finite element framework to illustrate its performance in several benchmark problems.

1. Introduction

Biofilms are our daily accompaniment, they can be found on teeth, contact lenses, drainpipes or medical devices and are one of the oldest and most successful forms of life on earth [124,113,142,43]. The term 'biofilm' describes aggregations of microorganisms embedded in a highly hydrated, self-produced matrix of extracellular polymeric substances (EPS). The manifold definitions of biofilms in literature [16,23,97] agree in defining them as microbial communities attaching to interfaces including solid–liquid, gaseous–liquid, gaseous–solid, or liquid–liquid ones [98,144,30]. Depending on their environment in the sense of nutrient supply or hydrodynamical loading, biofilms reach a typical thickness in the order of 100 μm. A classical situation might be found in an industrial plant system with fluid-filled pipes: Microorganisms, initially floating in the fluid attach to the inner walls, where they are supplied with nutrients. They start to proliferate and produce EPS, a process which is commonly defined as biofilm growth. The direction and rate of growth is dominated by the mechanical environment, e.g., fluid flow of limiting geometrical conditions, and by the nutrient supply. Nutrient uptake causes a gradient within the biofilm. A higher nutrient concentration and thus intensified growth is located at the top of the biofilm whereas microorganisms progressively die off at the bottom, causing a mechanical degradation that results in biofilm sloughing [133,46,1,58].

While some biofilms are related to serious problems in medicine and industry, others have vital physiological functions or are used in a large variety of technical applications [99,143,96], for a more detailed overview we refer to the recent review by Böl et al. [10]. Understanding how biofilms grow and affect their environment is a key issue to minimise the related risks and

* Corresponding author. Tel.: +49 5313917052.
E-mail address: m.boel@tu-bs.de (M. Böl).

http://dx.doi.org/10.1016/j.cma.2014.01.001
0045-7825/

exploit the technical possibilities. The development of numerical tools to predict biofilm growth characteristics and life cycles could be an essential element in order to find new ways to deal with both, the positive and negative aspects of microbial biofilms.

1.1. Extracellular polymeric substances

Crudely simplified, biofilms are mainly composed of microorganisms and EPS. The latter protects the microorganisms and is responsible for most of the biofilm's mechanical and physical properties such as density, porosity, or water content [40,43]. Following [146], EPS are composed of polysaccharides [132], extracellular proteins [92], extracellular DNA [136,24,29], and lipids [47,119]. Although the EPS constitution varies, their main constituents are in most cases neutral or polyanionic polysaccharides. Some of the aforementioned macromolecules enable the cohesion and adhesion of biofilm thus building complex three-dimensional EPS networks. Following [91], three types of binding forces play a key role in biofilm stability: Dispersion forces, electrostatic interactions, and hydrogen bonds. Particularly multivalent cations can enhance the strength of the network [131,2,59]. Accordingly, the mechanical characteristics of biofilms can be influenced by controlling the corresponding bonding forces [70,69,149], the interested reader is referred to the review by Böl et al. [10]. The complex and sophisticated microstructure provides biofilms with mechanical stability [41–43] to withstand external loads such as hydrodynamic and shear forces.

1.2. Biofilm formation and growth

The life cycle of biofilms, coarsely separated into the phases of formation, maintenance and erosion, is an ongoing dynamic process, cf. [131]. The first step of biofilm formation is the contact of microorganisms with the substratum. Thereby a layer of organic and inorganic substances develops and the microorganisms gradually form a reversible link to the surface [30]. This process strongly depends on the environment conditions [104,41,88,112], the microorganisms [101,5], as well as the surface characteristics [104,14,95]. In a further step the initially reversible connections become irreversible due to physicochemical interactions [13]. Then, microcolonies form and genetic changes inside the microorganisms lead to an enhanced production of EPS [141,131]. By this means and due to additional microorganisms settling from the liquid phase [77] the biofilm grows, while simultaneously channels arise [68,67]. The final step in the biofilm life cycle is the detachment of cells or clusters, mainly triggered by high hydrodynamic conditions. These cells and biofilm parts may again attach to a substratum thus restarting the live cycle [120,131].

The model presented herein focusses on the second step, in which cells proliferate and produce EPS so that the biomass increases by an uptake of nutrients. A thorough understanding and modelling of this step is critical in order to deal with the next steps such as sloughing and detachment.

1.3. Models of biofilm growth and development

Over the last decades extensive experimental effort has been devoted to study biofilm structure and formation. In parallel, the interest in modelling has strongly increased. The modelling concepts can coarsely be divided into two main types: *discrete* and *continuum approaches*. The discrete approach comprises *cellular automata* (CA) and *individual-based models* (IbM). CA are based on the idea that a (discrete) assembly of cells is allowed to change according to a set of rules. Each cell can take a state from a given set which changes according to prescribed rules depending on the cell's own state and that of its neighbours, for more details see e.g., [134,150,121]. CA modelling was applied in different biological and non-biological fields. With focus on biological growth modelling, Schindler and Rataj [122], Fujikawa [45], and Schindler and Rovensky [123] applied a diffusion-limited aggregation model [148] and random-walk models to describe biological community growth. However, these models were quite limited as they did not feature basic effects as e.g., nutrient dependence. A more realistic model for colony growth was presented by Ben-Jacob et al. [8], who included microorganism growth in a substrate gradient field. Based on studies by Colasanti [22], the first application of CA in biofilm modelling was realised in a study by Wimpenny and Colasanti [145]. Since that time the use of CA models in biofilm research increased, reaching from two-dimensional [53–55,61,62,80–83,85,107,109] to more complex three-dimensional approaches [107,108,100,15]. The basic idea of the second discrete type of modelling concept, IbM, is the relation of microscopic entities (cell) to the characteristics of macroscopic systems (biofilm). The main difference to CA models is that all processes run at the individual cell level and not at a predefined grid. With respect to modelling of ecological aspects, IbM were developed in various ways [25,60,51,52], thus providing tools to simulate a tremendous range of scenarios including cell division and death, substrate uptake, heterogeneity, detachment, maintenance, disinfection, metabolism, or multi-species consortia [71–73,106,105,152–154,151,27,26,3,49,78]. Both discrete concepts, CA and IbM, are powerful tools that can be found in ecological, social, economic, demographical, and political sciences, see [52] and references therein. They are still an active field of research and the interested reader is referred to the critical reviews e.g., by Wimpenny and Colasanti [145], Grimm [51], Picioreanu et al. [110], Grimm et al. [52], Ferrer et al. [39], Laspidou et al. [79], and Wang and Zhang [138].

The rules controlling the behaviour of discrete models act on a local inter-individual level and can hardly describe *global* relationships between the individuals. With application to mechanical problems, which are classically formulated as field equations, this poses a drawback. In this regard continuum-based models are more convenient. As their name implies, they