LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach(s)	**Supervisor(s)**
ir. Francisco Arraez	Prof. dr. ir. Paul Van Steenberge Prof. dr. ir. Dagmar R. D'hooge

Strength of modelling tools for the design and optimization of surface-initiated radical polymerization processes

Aim

Development of a computer model for the study of surface-mediated reversible addition-fragmentation chain transfer polymerization of methacrylate monomers.

Justification

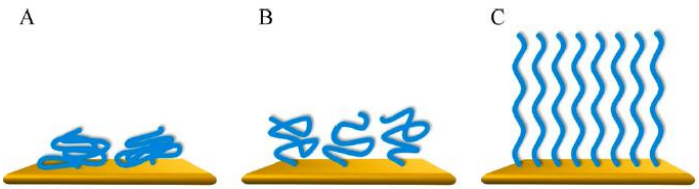

Figure 1: Three regimes of surface-tethered polymer chains: A) mushroom, B) brush-like, C) brush.

Surface-tethered polymers are a class of polymeric assemblies in which the individual polymer chains are tethered to planar or curved surfaces by at least one chain end. Modification of surface properties with the introduction of polymer chains allows for various applications including the production of coatings for corrosion protection, novel adhesive materials, protein-resistant biosurfaces, chemical lubricants, and polymer carriers for controlled-release of active compounds.

Reversible addition-fragmentation chain transfer (RAFT) polymerization is one of the main approaches to synthesizing polymer chains on surface with well-established structure and polymer composition as well as controlled molar mass and narrow molar mass distributions over a wide range of monomers. Upon using RAFT polymerization, the synthesis of polymer brushes can be conducted by anchoring either a radical source (initiator) or the chain transfer agent (CTA) on the surface, although the latter option is the most widely used and more common approach.

One of the most important challenges to deal with during the preparation of polymer layers on surface is to have complete information regarding important characteristics such as molar mass and dispersity of the tethered polymers as well as the variation of polymer layer thickness as a function of polymerization time and grafting density. This information cannot be easily accessed simply by conducting experimental studies which only allow the determination of average properties of free polymer chains in solution. However, this limitations can be circumvented through a combination of advanced computational modeling techniques with meticulous experimental analysis and the main goal of this project is to develop a computational tool based on the Method of Moments to account for the design of polymerization system aiming at optimal process conditions. This code has to be able to account for average properties of polymer chains either in solution or tethered to a surface.

Program

1. Concise literature review on RAFT polymerization technique for the optimal synthesis of polymer brushes as well as modeling strategies of surface-initiated polymerization processes.
2. Extension of a pre-existing computer code based on the Method of Moments to account for surface-tethered polymer chain synthesis via living surface-tethered polymerization via RAFT mechanism.
3. Validation and benchmarking of the code in 2 against experimental data obtained at the Laboratory for Chemical Technology as well as data reported in the literature.