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SIMULATION OF CONFORMATIONAL AND HYDRODYNAMIC PROPERTIES OF DENDRIMER-LIKE POLYMERS UNDER FLOW

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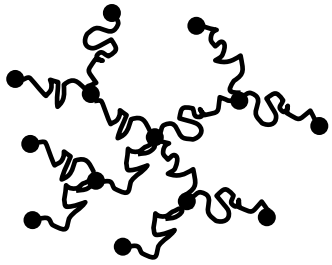
Dendrimers are highly and regular branched macromolecules that have attracted much attention due to their wide range of applications like catalysis, molecular recognition or drug delivery. Dendrimer-like star-branched polymers are a class of dendritic polymers, the first synthetic example dating back to 1995 (see the review [1] on the topic). These polymers exhibit molecular features similar to those of regular dendrimers, such as the presence of a central core, a precise number of branching points and many terminal functions. However, branches of regular dendrimers comprise a few atoms whereas dendrimer-like polymers present macromolecular chains between their branching junctions, as illustrated in the following sketch:



We show the dependence of the radius of gyration and the intrinsic viscosity on the number of generations as well as the expected shear flow behaviour of dendrimer-like polymer dilute solutions. For that purpose, polymers were modelled as beads connected by FENE springs and simulations were carried out by the Brownian dynamics algorithm, including hydrodynamic interaction, implemented in our public-domain program BROWFLEX [2]. Since several mathematical approaches can be used to build Brownian dynamics algorithms with hydrodynamic interaction, we also discuss the advantages and disadvantages found in working with them [3].

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