

Author's Accepted Manuscript

Molecular weight/branching distribution modeling of low-density-polyethylene accounting for topological scission And combination termination in continuous stirred tank reactor

Nazila Yaghini, Piet D. Iedema



www.elsevier.com/locate/ces

PII: S0009-2509(14)00197-3
DOI: <http://dx.doi.org/10.1016/j.ces.2014.04.039>
Reference: CES11621

To appear in: *Chemical Engineering Science*

Received date: 24 February 2014

Revised date: 4 April 2014

Accepted date: 25 April 2014

Cite this article as: Nazila Yaghini, Piet D. Iedema, Molecular weight/branching distribution modeling of low-density-polyethylene accounting for topological scission And combination termination in continuous stirred tank reactor, *Chemical Engineering Science*, <http://dx.doi.org/10.1016/j.ces.2014.04.039>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Molecular weight/branching distribution modeling of low-density-polyethylene accounting for topological scission and combination termination in continuous stirred tank reactor

Nazila Yaghini^a, Piet D. Iedema^{a,b}

^a Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, the Netherlands, yaghini.nazila@gmail.com, p.d.iedema@uva.nl

^b Dutch Polymer Institute DPI, PO Box 902, 5600 AX Eindhoven, the Netherlands

Abstract

We present a comprehensive model to predict the molecular weight distribution (MWD)¹, and branching distribution of low-density polyethylene ($ldPE$)², for free radical polymerization system in a continuous stirred tank reactor ($CSTR$)³. The model accounts for branching, by branching moment or *pseudo distributions*. The common free radical polymerization reactions including chain scission have been considered in the model. *Non-linear* or the so-called *topological* scission has been modeled using approximate *fragment length distributions* derived from scission, applied to branching topologies. To model the distributions, the Galerkin-FEM method based on the same principles as PREDICI® has been applied and implemented in MATLAB®. The fundamental numerical problem arising from topological scission has been solved. Thus, the model provides more accurate results, allowing a precise comparison to earlier results and to Monte Carlo simulations.

Keywords:

Free radical polymerization, Reaction engineering, Molecular architecture design, Product design, Galerkin FEM, Hypergeometric distribution

* Corresponding author. Faculty of science (HIMS); POSTBUS 94157; 1090 GD Amsterdam; Tel.: +31-20-525-6484; E-mail address: P.D.Iedema@uva.nl

¹ Molecular Weight Distribution

² low density PolyEthylene

³ Continuous Stirred Tank Reactor

Download English Version:

<https://daneshyari.com/en/article/6590999>

Download Persian Version:

<https://daneshyari.com/article/6590999>

[Daneshyari.com](https://daneshyari.com)