Available online at www.sciencedirect.com
ScienceDirect
Computers and Chemical Engineering 31 (2006) 51–65
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

Modeling and analysis of a plant for the production of low density polyethylene

M. Häfele[a], A. Kienle[b,*], M. Boll[c], C.-U. Schmidt[d]

[a] *Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany*
[b] *Chair for Automation/Modeling, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 6, 39106 Magdeburg, Germany*
[c] *BASF AG, 67056 Ludwigshafen, Germany*
[d] *Basell Polyolefine GmbH, 50387 Wesseling, Germany*

Received 9 August 2005; received in revised form 2 May 2006; accepted 4 May 2006
Available online 19 June 2006

Abstract

In this paper a detailed dynamic mathematical model of a plant for the production of low density polyethylene (LDPE) is derived. Besides the main part, a tubular reactor, the plant comprises compressors, heat exchangers and material recycles. The dynamic model for the overall system consists of differential, partial differential and algebraic equations. For the numerical solution with the simulator DIVA, this system is transformed into a system of differential and algebraic equations. For the transformation an adaptive finite difference scheme is used. With this mathematical model, the influence of the reactor wall and the influence of the material recycles on the plant dynamics is studied. In particular, it is shown that the reactor wall due to its high thermal capacity dominates the time constant of the stand alone reactor. By closing the material recycles the time constant is significantly increased. In addition, the recycles give rise to intricate nonlinear behavior.

Keywords: Dynamic model; Simulation; Discretization; Adaptive method of lines; Polymerization; Low density polyethylene; Tubular reactor; Method of moments

1. Introduction

Low density polyethylene is one of the most often produced polymers in the world. Its production takes place in a tubular reactor at high pressures. Fig. 1 shows the simplified flow-sheet diagram of a typical process which is considered subsequently. Besides the main unit, the tubular reactor with several different coolant cycles, the plant consists of two compressors, two separators, some heat exchangers, mixers, a valve and two material recycles. The plant is operated at very high pressures in between 2000 and 3000 bar at the inlet. Because of the high pressure, the thickness of the reactor wall is of the same order as the inner diameter of the tube. Also temperature is at a high level in a range of 400–600 K due to the exothermicity of the reaction. The reaction is started by adding initiators to the monomer. Very often peroxides are used as radical donators. Depending on the temperature, peroxides decompose into radicals and these radicals initiate the chain growth reaction. This reaction step is highly exothermic. To remove the reaction heat, different coolant cycles are used. Usually the tubular reactor for the production of LDPE is very long (>1000 m). Despite of the length of the reactor, conversion is very low. The conversion in the tubular reactor is only about 25–35%. Hence, flash units are used to separate the unreacted monomer from the product. The product is withdrawn and the unreacted monomer recycled. There are two material recycles, operated at the pressure, to which the flash units expand the flux.

The tubular reactor comprises different coolant cycles. Their cooling capacity can be adjusted independently by changing the throughput. The coolant cycles can be operated co- or counter current wise. Usually, right after an initiator injections there are two cycles which are operated at a higher temperature level. The subsequent two are operated at a lower level. For the derivation of the detailed dynamic mathematical model, the coolant cycles are used to divide the tubular reactor into modules. Four modules build up one section, the sections are bounded by the initiator injections and reactor boundaries. In other words, the reactor has four injection sections, which themselves can be divided into four coolant cycles.

* Corresponding author. Tel.: +49 391 6110 369; fax: +49 391 6110 515.
E-mail address: kienle@mpi-magdeburg.mpg.de (A. Kienle).

0098-1354/$ – see front matter
doi:10.1016/j.compchemeng.2006.05.001

Nomenclature

A	area
c_p	heat capacity
Δh_{reac}	heat of reaction
d	diameter
DB	double bonds
E	radiation energy
Gr	Grasshof number
I	initiator
J	total number of reactions
k	overall heat transfer coefficient, reaction rate constant
LCB	long chain branching
$\dot{m}$	mass flow
$\dot{m}_A$	mass flow through area A
M	monomer, molar mass
N_C	number of components
Nu	Nusselt number
P	polymer
P_z	centrifugal average
Pr	Prandtl number
$\dot{Q}$	heat flux
r	radius, reaction rate
R	radicals, overall heat transfer coefficient
Re	Reynolds number
s	thickness
SCB	short chain branching
t	time
T	temperature
U	perimeter
υ	velocity
w	weight fraction
X	modifier
z	axial coordinate

Greek letters

α	heat transfer coefficient
Δ	difference
ε	emissivity
λ	heat transport coefficient
μ_n	nth moment
ν	stoichiometric coefficient
σ	Stefan–Boltzmann constant
ϱ	density
ζ	pressure drop coefficient

Subscripts

0	initial condition
amb	ambience
A	flux, applied through cross section with area A
air	air
β	β-scission
bb	back biting
C	coolant
ex	external wall
hflash	high pressure flash
i	index of chain length
in	at inlet conditions
init	between two initiator injections
inner	at the inner reactor wall
iso	insulation
j	index of reactions
liq	liquid phase
ll	laminar layer
m	logarithmic mean
M	monomer
ν	index for initiators
outer	at the outer reactor wall
p	propagation
rad	radiation
rem	reminder of the tube
res	residence time
R	reactor
RX	modifier radical
sec	secondary living polymer
st	steel
sl	slime layer
tc	termination due to combination
td	termination due to disproportion
th	thermal
tr	transfer
υ_{ap}	vapor phase
W	wall
X	modifier

Superscripts

P	dead polymer
R	living polymer

A simplified flow sheet of a polyethylene production is depicted in Fig. 1. In a typical polyethylene plant, more than 15 different grades of LDPE, differing in their physical properties, are produced. Since stocking costs are huge, the strategy is to produce just in time what is required by marked demands. So the plant has to undergo frequent grade changes. Moreover, the plant is usually connected in a production network. Up- or downstream processes influence the throughput of the plant directly. Despite of changes in throughput, product quality, depending on, e.g. the chain length distribution, has to remain within the product specifications. For the optimization of grade or load changes, a detailed dynamic model that contains the necessary information on the product properties has to be used.

In literature, one can find many studies dealing with the steady state behavior of such a plant (e.g. Kiparissides, Verros, & MacGregor, 1993; Zabisky, Chan, Gloor, & Hamielec, 1992) but only little investigation has been carried out using dynamic models. In those dynamic studies, usually only very simple and small models have been used (Asteasuain, Tonelli, Brandolin, & Bandoni, 2001; Kiparissides, Verros, & Pertsinidis, 1996).