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Dynamic simulation of a tubular reactor for the production of low-density polyethylene using adaptive method of lines

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

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

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Abstract

The dynamic mathematical model of a tubular reactor for the production of low-density polyethylene (LDPE) is introduced and simulation studies of a LDPE plant are presented. The plant consists of the tubular reactor, compressors, heat exchangers and material recycles. The overall model formulation comprises differential, partial differential and algebraic equations. This model formulation is transformed into a DAE system using an adaptive method of lines approach, where the grid points may change their position but their number remains constant. With this technique a solution on a standard PC is possible.

Keywords: Mathematical model; Dynamic simulation; Discretization; Adaptive method of lines; Polymerization; Low-density polyethylene; Tubular reactor

1. Introduction

Low-density polyethylene (LDPE) is one of the most often produced polymers in the world. The process has been established in the early 1970s. There are two reactor types where the polymerization is carried

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

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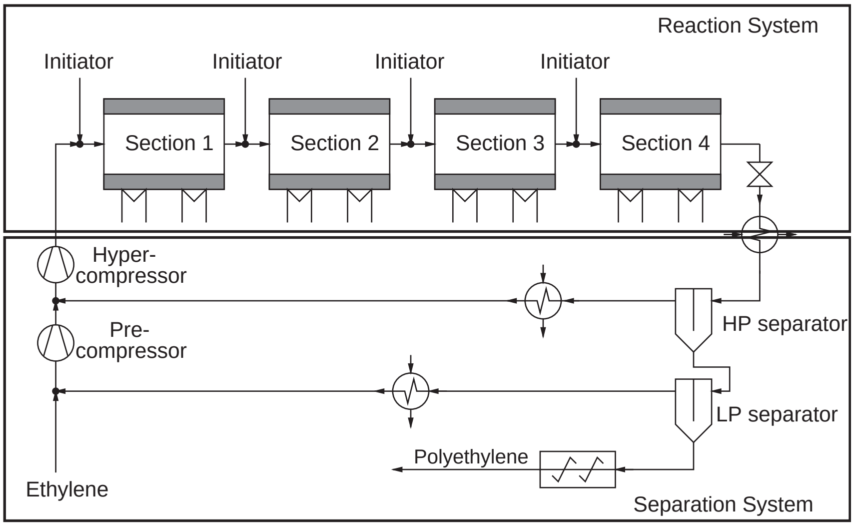

Fig. 1. Flow-sheet of the LDPE production plant.

out, an autoclave reactor, and a tubular reactor, which is considered here. Even though the process is well established, in literature there are only few studies available, which deal with the dynamic behavior of this process. The steady-state behavior has been examined in all the levels in detail [2,3], but for the analysis of the dynamic behavior only very simple models have been used so far [1].

A flow-sheet diagram of the process is depicted in Fig. 1. The plant consists of the tubular reactor and some peripheral units, such as compressors, separators, heat exchangers, mixers, a valve and two recycle lines. The operating conditions under which low-density polyethylene is produced, are quite extreme. The pressure at the reactor inlet is in between 2000 and 3200 bar and the temperature regime is in the range 400–600 K. Because of the high pressure, the thickness of the reactor wall is of the same order as its inner diameter. The reaction is initiated by free radicals, which are generated by decomposition of radical donators, i.e. initiators. Most often peroxides are used for that step. The subsequent chain growth reaction is highly exothermic. In order to remove the heat of reaction, these tubular reactors are not only very long (> 1000 m), but the injection of initiator is distributed along the tube. Nevertheless, only 30–35% of the monomer can be converted to polymer due to high exothermicity of the reaction. Therefore, unreacted monomer is separated from the polymer and recycled into the reactor. There are two recycle lines, one operated at higher pressure, the other one at almost ambient conditions.

For the derivation of the mathematical model equations, the tubular reactor is divided into 16 modules. Each of these modules comprises one coolant cycle, operated counter-current wise. Four modules build one section, different sections are bounded by the initiator feeds or the reactor boundaries itself.

Usually, such a plant is connected in a production network with up- and down-stream processes. These processes have influence on the throughput of the plant. Despite of changes in throughput, product quality, which is characterized e.g. by the melt flow index or the density, has to remain constant. Moreover, more than 15 different types of polyethylene are produced in such a plant. Since stocking costs are huge, the