Chemical Engineering Science 101 (2013) 674–685

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Model design of a class of moving-bed tubular gasification reactors

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HIGHLIGHTS

- Model reduction approach for two-phase moving-bed tubular gasification reactors.
- Reduction based on quasi-steady state gas-phase and stoichiometric assumptions.
- Tubular reactor represented as a train of N continuous stirred tank reactors.
- Number of tanks and their volumes are design degrees of freedom.
- Case example simulations show that reactor dynamics can be modeled with three tanks.

ARTICLE INFO

Article history:
Received 22 August 2012
Received in revised form
26 June 2013
Accepted 1 July 2013
Available online 24 July 2013

Keywords:
Model reduction
Moving bed
Multiphase reactors
Chemical reactors
Tubular reactor
Gasification reactors

ABSTRACT

The problem of modeling a class of two-phase moving-bed tubular gasification reactors by means of a lumped (finite-dimensional) representation is addressed in this paper. A model is designed, as simple as possible, in the light of a specific – experimental, equipment, operation, monitoring or control – design task and the uncertainty of the underlying kinetics and transport parameters. First, the enforcement of quasi-steady state (QSS) gas-phase assumptions and stoichiometric considerations followed by spatial finite-difference approximation plus interpolation leads to a representation of the tubular reactor as a train of N continuous stirred tank reactors (CSTRs). Then, the number of tanks and their volumes are chosen according to the modeling objective. The proposed approach is illustrated with a case example, studied before with experiments and PDE-based simulations, finding that the dynamics of the tubular reactor can be modeled with three CSTRs (9-ODE).

1. Introduction

The conversion of a carbonaceous solid fuel into a gaseous one (syngas or producer gas) has become an interesting alternative for power generation and energy conversion (Beér, 2007). A diversity of fluidized, entrained and moving-bed two-phase tubular reactors has been employed to carry out the reaction. A state-of-the-art description of the wide variety of gasification technologies is provided in the literature (Reed and Das, 1988; Basu, 2006; Higman and van der Burgt, 2008). This paper focuses on the moving-bed reactor, which has the advantage of enabling small-scale operations with a suitable trade off between product quality and variability of solid feed composition.

In two extensive studies (Amundson and Arri, 1978; Caram and Fuentes, 1982), according to the standard chemical reactor modeling plus space finite-differences discretization, it was established that in operation at maximum thermal efficiency a countercurrent moving-bed reactor exhibited the following behavior: (i) strong parametric sensitivity with respect to feed flows, (ii) traveling reaction front behavior, and (iii) three steady-state profile sets for a certain solid flow rate interval. These features were validated in subsequent experimental steady-state (Manurung and Beenackers, 1993; Reed et al., 1999; Zainal et al., 2002; Sheth and Babu, 2009) and transient (Reed and Markson, 1985; Barrio et al., 2001; Shwe, 2004) studies. In particular, Reed and Markson (1985) and Barrio et al. (2001) reported that: (i) two different steady-states were possible, one with reaction front close to the reactor solid phase inlet and high solid conversion, and the other one with front close to the exit and low conversion and (ii) either steady-state can be reached depending on the feed flow rate value. In an experimental study of a coal gasifier with PID temperature control (Chen et al., 2007), it was reported an initial transient response dominated by pyrolysis (due to the relatively high yields of H_2 and CH_4) followed by a response governed by char gasification (high measured concentrations of CO and CO_2). In view of Amundson and Arri (1978) study, it is not clear if the open-loop

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http://dx.doi.org/10.1016/j.ces.2013.07.001

operations are unique or not, and if they were or not close to bifurcation conditions.

Recently, simulation studies have been conducted for performance and parameter sensitivity evaluation of the biomass feed processes (Di Blasi, 2000, 2004; Rogel and Aguillon, 2006; Gobel et al., 2007; Grieco and Baldi, 2011) with models that: (i) constitute variations and/or refinements of the one developed by Amundson and Arri (1978) and (ii) yield rather good quantitative descriptions of experimental data. Among the refinements are: more components and reactions (two step pyrolysis finite kinetics), gas-phase quasi-steady-state (QSS) assumption, radial dependency of the profiles, thermal equilibrium between phases and use of computational fluid dynamics (CFD) tools. The models describe the experimental data with 8–15 and 5–12 percent deviations for absolute temperature and gas effluent concentrations, respectively.

Even though these models suffice for process design and redesign, they may be unduly high dimensional and stiff due to the absence of gas-phase QSS assumptions (Gobel et al., 2007), and of stoichiometry-based partition of species (Aris, 1965; Feinberg, 1977). The availability of reduced order models should: (i) facilitate studies on the key multiplicity and stability issues and (ii) enable the development of tractable advanced monitoring and control schemes, in the understanding that the stability, estimation and control theory for infinite dimensional systems lags quite behind the one for finite dimensional ones. These considerations motivate the scope of the present study: the development of a reduced-order modeling framework for tubular moving-bed gasification reactors.

The methodological assumptions used in this paper are based on the idea that, in constructive control (Sepulchre et al., 1997; Krstic et al., 1995), the choice of model itself is a design degree of freedom that can be effectively exploited to devise nonlinear observers and (advanced and conventional) controllers for CSTRs (Lopez and Alvarez, 2004; Diaz-Salgado et al., 2012; Schaum et al., 2012), for drying distributed systems (Martinez-Vera et al., 2010), and (distributed-like) staged systems (Castellanos-Sahagun et al., 2006; Fernandez et al., 2012).

In this paper, the problem of designing the model, in the light of a specific objective, for a class of two-phase moving-bed tubular gasification reactors is addressed. Among the modeling objectives are: experimental, equipment, operation, monitoring and control design. The problem consists in developing the simplest possible lumped (finite-dimensional) representation of the syngas tubular reactor such that the particular modeling objective is met with the smallest number and weakest coupling of ordinary differential equations (ODEs), relative to the uncertainty of the kinetics and transport parameters and the prescribed model accuracy.

First, the enforcement of quasi-steady state (QSS) gas-phase assumptions and stoichiometric considerations, followed by spatial finite-difference (FD) approximation plus interpolation leads to a reduced order dynamical model of the reactor, that is interpreted as a train of N continuously stirred tank reactors (CSTRs) with backmixing. The number of tanks and their volumes are regarded as design degrees of freedom and chosen according to the modeling objective. The proposed approach is applied to a case example studied previously with experiments (Manurung and Beenackers, 1993) and simulations (Di Blasi, 2000), finding that reactor dynamics can be adequately modeled with three CSTRs (9-ODE).

2. Reactor modeling problem

In this work, a continuous moving-bed tubular gasifier reactor (depicted in Fig. 1) is considered where solid-to-gas fuel conversion occurs according to a multicomponent reaction network in the gas and solid phases. Two feed streams are connected to the reactor, one at the top with the solid fuel particles (coal, municipal waste or wood pellets, assumed mono-disperse), and the other one supplying the gasification agent (air, oxygen, steam or a mixture of them) either from the top or from the bottom. The reactor is equipped with two exit streams, one with the unreacted solid particles (ash and char), and the other with the syngas product. Without restricting the approach, this paper is circumscribed to the case of downdraft operation with concurrent feed flow pair (Fig. 1).

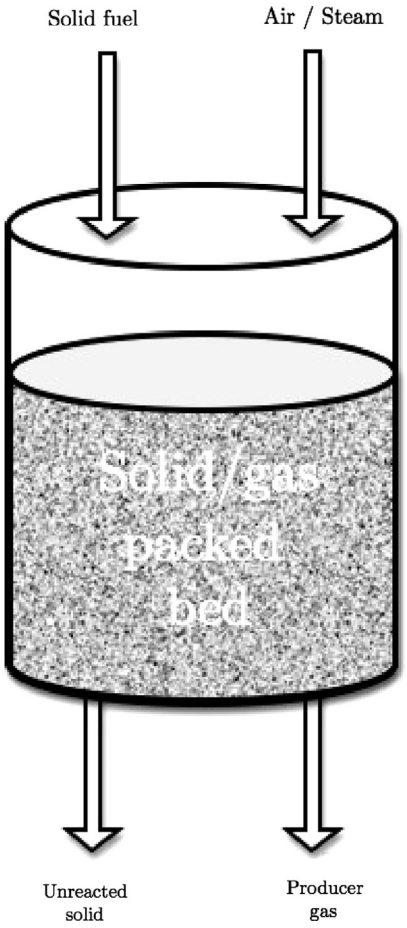

Fig. 1. Concurrent moving-bed tubular gasifier.

2.1. Reactor distributed system

For the modeling purpose at hand, let us regard that solid-to-gas fuel conversion occurs through a pseudo-homogeneous reaction network of m reactions, n_π^R reactive components, and n_π^I inert components ($n_\pi = n_\pi^R + n_\pi^I$) in the π (gas or solid) phase, according to the following expression in stoichiometry-oriented form (Aris, 1965):

$$s_{1,j}^{\pi}\Omega_1^{\pi} + \cdots + s_{n_\pi^R,j}^{\pi}\Omega_{n_\pi}^{\pi} = 0, \quad j = 1,\ldots,m \tag{1a}$$

$$\mathbf{R}_j(\mathbf{A},T), \quad \Delta H_j, \quad \pi = g,s$$
$$g = gas, \quad s = solid$$
$$\mathbf{A}_\pi = [A_1^\pi, A_2^\pi, \ldots, A_{n_\pi}^\pi]^T \tag{1b}$$

$$\mathbf{A} = [\mathbf{A}_g^T, \mathbf{A}_s^T]^T, \quad \mathbf{T} = [T_s, T_g]^T \tag{1c}$$

where Ω_i^π is the i-th component in the π phase, $s_{i,j}^\pi$ is the stoichiometric coefficient of the i-th component Ω_i^π in the j-th