3rd IFAC/IEEE CSS Workshop on Control of Systems Governed by Partial Differential Equations CPDE and XI Workshop Control of Distributed Parameter Systems, CDPS 2019, May 16-18 2019 Oaxaca, Mexico

Modeling, estimation, and control of spatially distributed heterogeneous tubular chemical reactors

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Due to their ability to handle strongly exothermic reactions with high reaction rate per unit volume (Froment et al, 2006), heterogeneous fixed and moving bed spatially distributed tubular reactors are employed in a diversity of important industrial processes (Jensen and Ray, 1982; Basu, 2013; Yuan et al., 2015), among them are carbon monoxide and ethylene oxidation, carbon monoxide methanation, ammonia synthesis, polymerization, crystallization, biomass anaerobic digestion, catalytic pyrolysis, coal and biomass gasification and combustion. These reactors, underlain by a complex interplay of multicomponent reaction and convective-dispersive transport, may exhibit typical nonlinear phenomena (Elnashaie and Grace, 2007) -such as steady-state (SS) multiplicity, bifurcation, and limit cycling- (Hubbard and West, 1995; Seydel, 2010; Kielhöfer, 2012) that must be regarded in safety, scaleup, operation, monotoring, and control designs (Elnashaie and Elshishini, 1993; Morud and Skogestad, 1998; Dochain, 2018).

These reactors are modeled by (typically, 2 to 17-profile) nonlinear partial differential equations (PDEs) which are numerically solved with standard (high-order) and reduced-order PDE-to-ordinary differential equation (ODE) spatial discretization schemes. Sice the computational load depends on the number of equations and their ill-conditioning, reduced order modeling is important to perform efficient off-line process (Luyben, 2001) as well as tractable on-line monitoring and control (Christofides, 1998; Li and Christofides, 2008) designs.

Mostly for single and two-profile homogeneous and heterogeneous tubular reactors, multiplicity assessments have been done with bifurcation analysis (Golubitsky and Shaeffer 1985; Kuznetsov, 1998; Seydel, 2010) through numerical continuation (Keller, 1977; Doedel et al., 1991), using a diversity of discretization schemes (Razon and Schmitz, 1987): finite differences (FD) (Varma and Amundson, 1973; Juncu and Floarea, 1995), single and multiple-finite element (FE), orthogonal collocation (OC) (Jensen and Ray, 1982; Liu and Jacobsen, 2004), and proper orthogonal decomposition (POD) Galerkin (Bizon et al, 2008) spatial discretization.

It has been reported that over-discretization can alter the PDE dynamics (Jensen and Ray, 1982, Lafon and Yee, 1996; Liu and Jacobsen, 2004), in the sense of limit set induction or elimination, and that the combination of steep profiles with global basis functions leads to excessive or intractable computability by ill-conditioning (Jensen and Ray, 1982, Bizon et al, 2008). Few continuation-based multiplicity assessments have been done, not without computational difficulties, for many (6 to 19)-profile tubular reactors (Amundson and Arri, 1978; Zitlalpopoca-Soriano et al., 2010), all of them have used 50 to 200-node mesh spatial FD discretizations. The heavy computational load grows rapidly with the number of equations, their ill-conditioning, and the intricateness of the multiplicity pattern (Allgower and Georg, 1990; Shampine, 1993).

The direct application of PDE solver-based modeling schemes is questiond by the cell modeling approach (Deans and Lapidus, 1960; Levenspiel and Bischoff, 1964; Deckwer, 1974) because: (i) the pseudo-homogeneity assumption of a PDE model breaks down at bed particle and/or eddy scale, and (ii) the use of a discretization other than first-order FD induces unduly ODE ill-conditioning due to spurious spatial interaction induction (Rutzler, 1980). On the basis of 8-to-20 cell models, 8 to 29-SS tubular reactor multiplicity has been reported (Sinkule et al., 1976; Hegedus et al., 1977; Wagialla and Elnashaie, 1995), and it is not known if the discretized models contain or not spurious SSs.

The need of having more systematic means to address the reduced-order modeling problem of hetergogeneous tubular reactors motivate the scope of the present presentation (Santamaria-Padilla et al, 2018; Badillo-Hernandez et al., 2013, 2019): the development of a methodology to efficiently describe with a reduced-order model the nonlinear dynamics of many-component heterogeneous tubular reactors. The aim is to model steady-state (SS) multiplicity, bifurcation, robust stability, and transient behavior, with preclusion of PDE dynamics alteration by overlumping and of unduly overmodeling by underlumping. Efficiency (to be technically stated) is the ability to describe, quantitatively, up to kinetics-transport (KT) parameter and computation errors and with the smallest possible order, the PDE dynamics of the reactor.

First, the reduced-order modeling methodology is developed by combining notions and tools from nonlinear dynamics, numerical methods, and chemical reactor engineering. The notion of model reliability (Bizon et al., 2008) is stated as structural stability with respect to model order, and a definition of efficiency is introduced. The model order determination problem is casted as the solution of a set of equations, with solvability depending on the particular discretization scheme-reactor pair. The efficient model order is calculated with bifurcation analysis and continuation with respect to model order.

Then, the proposed reduced-order modeling approach for tubular reactors is illustrated and tested with a representative 13-profile moving bed gasification tubular reactor studied before with experiments (Barrio et al., 2001; Shwe, 2004; Perez et al., 2012; Olaleye, 2014) and PDE simulations (Di Blasi, 2000; Di Blasi & Branca, 2013; Badillo et al, 2013; Patra and Sheth, 2015; Mahapatra et al., 2016), and with multiplicity assessment as open problem. It is found that the reactor is robustly bistable, and can be described by a 30th-order model with considerably less equations than in previous related studies.

Finally, the on-line variant of the ODE modeling approach is employed to address the following problems based on temperature and feed flow measurements: (i) state (Badillo-Hernandez et al., 2017) and state-input estimation (Badillo-Hernandez et al., 2019), (ii) Peclet (convective-to-dispersive heat transport) number identification (Badillo-Hernandez et al., 2018), and (iii) stabilizing robust output-feedback control (Najera et al., 2015; Contreras et al., 2018).

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