Low order online modeling of a distributed syngas reactor

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Abstract: The problem of modeling the startup dynamic profiles of a spatially distributed syngas reactor with the least possible dimension model and one online temperature measurement is addressed. First, the PDE reactor model is discretized via finite differences with a nonuniform spatial mesh yielding a staged model of adjustable spatial-partition. The number of stages and the spatial-partition of the staged-model are heuristically chosen such that the steady-state behavior is adequately described in the light of kinetic-transport parameter and experimental uncertainty. Then, the dynamics of the resulting nonuniform staged model are restricted by the online measurement. The modeling approach is illustrated with a case example finding that the startup operation can be described using a model with 5 non-uniform stages, 15 ODEs and a suitably located sensor, in the understanding that the same description through offline equistage modeling requires 90 ODEs, and 2000 ODEs with a PDE solver.

Keywords: gasification reactor, low order model, distributed nonlinear dynamics.

1. INTRODUCTION

Developing energy sustainable systems, based on renewable fuels like biomass, is an imperious necessity nowadays. The syngas gasification reactor is a notable choice for bioenergy generation due to its high efficiency, wide variety of low cost available raw materials and its relatively simple operation. Modeling studies of syngas reactors are motivated by a diversity of reliability and energy efficiency issues that limits its wide commercial application (Shwe, 2016; Ruíz et al., 2013; Yun, 2012; Dasappa et al., 2011).

Gasification reactors can exhibit steady state (SS) multiplicity and bifurcation phenomenon according to classical (Amundson & Arri and Amundson, 1978; Caram and Fuentes, 1982) and recent (Ranzi et al. 2014; Badillo-Hernández et al. 2017b) studies. In consequence, the related stability problems of this kind of tubular reactors can be effectively solved within a global nonlinear framework through model-based operation design, as well as advanced estimation and control systems synthesis, for which low-dimensional models are desired. However, most of the recent modeling (Di Blasi 2000; Gobel et al., 2007; Rogel and Aguillon, 2006) studies have focused on local stable ignition steady state description by means of high order models (2000-7000 ODEs) obtained from the discretization of PDE reactor model with finite differences, finite volume and CFD packages.

With regard to the high dimensionality obstacle, previous studies on small scale packed bed syngas reactors have shown that: (i) the local dynamics around the ignition steady state of interest can be quantitatively described using a non-uniform mesh-based 3-to-5-stage model (9-to-15 ODEs) (Badillo-Hernández et al. 2013), (ii) the global bistable behavior can be qualitatively described with a 10-equistage model (30 ODEs), (iii) the startup operation can be quantitatively explained with a 30-equistage model (90 ODEs) (Badillo-Hernández et al. 2017b), and (iv) the temperature, concentration and flow spatial profiles (or effluent values) can be inferred by means of a geometric estimator of 6 (or 8) stages of uniform spatial-partition and 18 (or 24)-ODE, and two (or one) temperature sensors (Badillo-Hernandez et al., 2016, 2017a).

On the other hand, Baratti et al. 1993 designed an online model to estimate concentration in an experimental catalytic reactor with complex Langmuir-Hinselwood kinetics. This online model, driven by the experimental temperature measurement, was called open loop observer. In the bioreactors engineering literature, this kind of online models are called asymptotic observers (Dochain, et. al. 1992) and has been implemented for a coal fluidized bed gasifier (Botero et al., 2013).

These results in the light of the preceding offline and online modeling considerations motivate the scope of the present study: the development of a low order online modeling approach that: (i) matches or outperforms the online geometric estimator (Badillo-Hernandez et al., 2017a), and (ii) has a simpler online data processing scheme. This online modeling is performed on the basis of: (i) a heuristically chosen non-uniform spatial-partition of the staged model, and (ii) an online temperature measurement adequately located along reactor.

2. MODELING PROBLEM

The present study focuses on the pilot-scale moving bed tubular syngas reactor depicted in Figure 1 (with length L, transversal area A_r, and metal mass M_w), where pyrolysis-gasification-combustion reactions occur between the solid biomass (at mass rate M_{se} and temperature T_{se}) and air (at volumetric flow Q_{ge} and temperature T_{ge}) streams producing a solid mixture of char and ashes (with mass flow M_{sf}, density vector $\boldsymbol{\rho}_{sf}$, and temperature T_{sf}) and a combustible syngas stream (with volumetric flow Q_{gf}, concentration vector $\boldsymbol{C}_{gf}$, and temperature T_{gf}) with useful caloric value. The solid phase is composed of two ($n_s = 2$) species: biomass (B) and char (C), and the gas phase has $n_g = 8$ species: $O_2, H_2, CO, CO_2, H_2O, CH_4, Tar, N_2$.

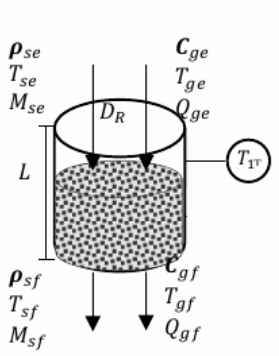

Fig. 1 Moving bed syngas reactor.

Let us recall the first-principles based distributed model (1) of the syngas reactor previously developed (Badillo-Hernandez et al. 2013, 2017b). This model has $n_s + 1$ partial differential equations (PDEs) (1d-e) and $n_g + 2$ boundary value ordinary differential equations (BVODEs) (1a-c) in dimensionless form.

$$0 \approx -\partial_z\left[v_g\, c_G(\tau)\right] + \boldsymbol{m}_g^T \boldsymbol{r}\,(\boldsymbol{c},\tau) \quad (1a)$$
$$0 = c_{C0}\partial_z v_s + W_{ab}\,\boldsymbol{r}(\boldsymbol{c}_s,\tau) \quad (1b)$$
$$0 \approx -\partial_z[v_g \boldsymbol{c}_g] + \boldsymbol{S}_g \boldsymbol{r}(c,\tau) \quad (1c)$$
$$\partial_t c_s = -\partial_z[v_s \boldsymbol{c}_s] + W_{ab}\boldsymbol{S}_s \boldsymbol{r}(\boldsymbol{c},\tau) \quad (1d)$$
$$\partial_t \tau = h_T^{-1}(\boldsymbol{c}_s)\{\partial_z[\delta\,\kappa(\tau)\partial_z\tau - v_H(\boldsymbol{v},\boldsymbol{c},\tau)\tau]$$
$$\partial_z[h_T(c_s)v_s]\tau - v(\tau)[\tau - \tau_w(t)] + W_{ab}\boldsymbol{\Delta}^T\boldsymbol{r}(\boldsymbol{c},\tau)\} \quad (1e)$$
$$y = \tau(z_y,t), \quad 0 < z_y < 1, \quad \partial_{zz}^2\underline{\tau}(z_y) \approx 0 \quad (1f)$$

with boundary and initial conditions

$$z = 0{:}\ \boldsymbol{c}_\theta(0,t) = \boldsymbol{c}_{\theta e}(t), \quad v_\theta(0,t) = v_{\theta e}(t), \quad \theta = s,g$$
$$\delta\kappa(\tau)\partial_z\tau = v_h(\boldsymbol{c},\tau)[\tau - \tau_e(t)] \quad (1g)$$
$$z = 1{:}\ \partial_z\tau = 0;\ t = 0{:}\boldsymbol{c}_s(z,0) = \boldsymbol{c}_{so}(z),\ \tau(z,0) = \tau_o(z) \quad (1h)$$

where

$$\boldsymbol{c} = (\boldsymbol{c}_s^T, \boldsymbol{c}_g^T)^T, \quad \boldsymbol{c}_s = (c_1^s, c_2^s)^T, \quad \boldsymbol{c}_g = (c_1^g, \dots, c_8^g)^T$$
$$\boldsymbol{r}(\boldsymbol{c},\tau) = (r_1, \dots, r_{n_R})^T(\boldsymbol{c},\tau), \quad \boldsymbol{\Delta}^T = (\Delta_1, \dots, \Delta_{n_R})^T$$
$$\boldsymbol{m}_g^T = \boldsymbol{S}_g 1_{ng}, \quad h_T(\boldsymbol{c}_s) \approx c_{pS}c_S(\boldsymbol{c}_s), \quad \kappa(\tau) = \frac{K(T_r)}{K(T)}, \quad \delta = \frac{1}{Pe}$$
$$v(\tau) = St_w\mu(\tau), \quad St_w = \frac{Lh_w(\tau_r)}{H_{sr}V_{sr}}, \quad \mu(\tau) = \frac{h_w(T_r\tau)}{h_w T_r},$$
$$v_h(\boldsymbol{v},\boldsymbol{c},\tau) = W_{ab}v_g c_{pG}c_G(\boldsymbol{c},\tau) + v_s c_{ps}c_s(\boldsymbol{C_s}), \boldsymbol{v} = \left(v_s, v_g\right)^T$$

The definitions of PDE model variables and parameters are listed in Table 1. In this study, we consider that a temperature measurement y is available at the axial location z_y, with the largest slope change, employed in industrial temperature controllers (Bashir et al., 1992). The distributed model (1) is set with the reference nominal parameters used in previous simulation studies (Di Blasi 2000, Badillo-Hernandez et al. 2013) for a pilot-scale experimental reactor (Manurung & Beenackers, 1993).

In compact notation, the PDE reactor model (1) is written as

$$\partial_t\boldsymbol{\chi} = F(\boldsymbol{\chi},\boldsymbol{u},\boldsymbol{p}), \quad \chi(0) = \chi_o, \quad \boldsymbol{\Omega} = G(\boldsymbol{\chi},\boldsymbol{u}) \quad (2a\text{-}b)$$

where

$$\pi \coloneqq (\boldsymbol{\chi}^T, \boldsymbol{\Omega}^T)^T \quad (2c)$$
$$\boldsymbol{\chi}(t) = [\boldsymbol{c}_s(z,t), \tau(z,t)]^T, \quad \boldsymbol{\Omega}(t) = \left[\boldsymbol{c}_g(z,t), \boldsymbol{v}(z,t)\right]^T$$
$$\boldsymbol{u} = (v_e^T, c_e^T, \tau_e, \tau_a), \boldsymbol{v}_e = (q_{se}, q_{ge})^T/A_R, c_e = (c_{se}, c_{ge})^T \quad (2d)$$

$\boldsymbol{\chi}$ (or $\boldsymbol{\Omega}$) is the solid concentration-temperature profile (or quasi-static gas concentration-axial velocity) pair, F and G are the integro-differential operators, and $\boldsymbol{p}$ is the vector of transport-kinetics parameters. The exogenous input vector $\boldsymbol{u}$ contains the feed flows (Q_{se}, Q_{ge}), concentrations (c_{se}, c_{ge}), the feed temperature (τ_e), and the wall temperature (τ_w).

Table 1. Nomenclature

t	Time
z	Axial position
τ	Temperature
τ_w	Mass metal Temperature
c_i^θ	Concentration of the $i-th$ component, θ: s, g
W_{ab}	$Air-biomass$ feed ratio
$\boldsymbol{m}_g$	Mass net generation vector in gas phase
v_θ	Velocity, θ: g, s
v_H	Effective heat convective flux
κ	Effective thermal conductivity of the bed
C_θ	Total molar concentration, θ: g, s
$C_{p\theta}$	Specific heat capacity, θ: g, s
S_θ	Stoichiometric submatrix, θ: g, s
r_j	$j-th$ reaction rate
Δ_j	$j-th$ heat of reaction
μ	Wall heat transfer coefficient
δ	Heat dispersion number ($Pe = 1/\delta$)
y	Temperature measurement at the axial location z_y

Now, consider the parametric uncertainty and unmodeled dynamics of the distributed model (1-2), so that, we define the actual dynamics of the reactor

$$\partial_t\xi = H(\chi_a,\xi,\boldsymbol{u},\boldsymbol{p}), \quad (3a)$$
$$\partial_t\chi_a = F(\chi_a,\boldsymbol{u},\boldsymbol{p}) + F_m(\chi_a,\xi,\boldsymbol{u}) \quad (3b)$$
$$\pi_a{:} = (\chi_a^T,\xi^T)^T \quad (3c)$$

χ_a (or ξ) is the actual (or not modeled state), F_m contains the transport-kinetics and parasitic dynamics error in (1). Consequently, a modeling error ε_p, between the nominal description through of PDE model (1-2) and the actual response of the reactor (3), arises according to the expression:

$$\varepsilon_p = ||\,\tilde{\pi}(t)|| > 0, \quad \tilde{\pi}(t) = \pi_a(t) - \pi(t) \quad (4)$$

2.1 Off-line staged model

Following standard PDE numerical solution strategies, the application, over $N+1$ uniform spatial intervals, of a finite difference or element method to the infinite-dimensional PDE model (2) yields the finite-dimensional n_x-ODE staged model:

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{p},\boldsymbol{\sigma}),\ \boldsymbol{x}(0) = \boldsymbol{x}_0, \quad \boldsymbol{x} \in X \quad (5a)$$
$$\boldsymbol{w} = \boldsymbol{g}(\boldsymbol{x},\boldsymbol{u}),\ \boldsymbol{w} \in W \quad (5b)$$
$$y = \tau_i, \quad i \in [1,N], \quad \Delta^2\tau_i \approx 0 \quad (5c)$$
$$\chi_N(t) = I_N^\chi[\boldsymbol{x}(t),\boldsymbol{u}(t)],\ \Omega_N(t) = I_N^\Omega[\boldsymbol{w}(t),\boldsymbol{u}(t)] \quad (5d)$$
$$\pi_N = (\chi_N^T, \Omega_N^T)^T$$
$$\boldsymbol{\sigma} \coloneqq \{N,\boldsymbol{\zeta}\}, \quad \boldsymbol{\zeta} = \{z_1, \dots, z_N\}, \quad 1 < i < N \quad (5e)$$
$$z{:}\ z_0 = 0 < \dots\dots < z_k < z_N < z_{N+1} = 1$$

where

$$dim\,\boldsymbol{x} = N(n_s+1) \coloneqq n_x,\ dim\,\boldsymbol{w} = N(n_g+2) \coloneqq n_w \quad (5f)$$

$\boldsymbol{\sigma}$ is the *lumping set* with the two modeling degrees of freedom: i) the number of internal nodes N and ii) the spatial partition

$\boldsymbol{\zeta}$. The lumping set determines the complexity of the lumped staged model due to the linear dependency of state dimension on N (5f). $\boldsymbol{x}$ (or $\boldsymbol{w}$) is the dynamic (or quasi-static) state sequence in the bounded set X (or W), and I_χ (or I_Ω) is the interpolation operator that yields the continuous profile χ_N (or Ω_N) from the vector $\boldsymbol{x}$ (or $\mathbf{w}$).

The approximation error (ε_N) with respect to the PDE solution vanishes, in the sense of a suitable spatial-temporal norm ($|\cdot|$) [LeVeque, 2007], according to the expression:

$$lim_{N\to\infty}\,\varepsilon_N = 0,\quad \varepsilon_N > \varepsilon_{N+1},\ \varepsilon_N = |\tilde{\pi}_N(t)|, \tag{6a}$$

$$\tilde{\pi}_N(t) = \pi_N(t) - \pi(t),\qquad \pi_N = (\chi_N^T, \psi_N^T)^T \tag{6b}$$

meaning that the PDE dynamics (1) are the limiting dynamics of the N-stage model (4) in the sense that, as $N \to \infty$, the staged system (5) becomes the nominal PDE one (1-2). Without restricting the approach, PDE discretization with finite differences method will be considered. Henceforth, $\boldsymbol{\sigma}$ will be called the lumping set with N and $\boldsymbol{\zeta}$ as the number of stages and spatial partition, respectively, and the PDE discretization (5) will be referred to as N-stage model (N-SM). In the case of syngas reactors, the PDE solver are underlain by N_{pde}-SM (5) with N_{pde} ranging from 200 to 700 (Di Blasi, 2000, Shwe, 2004).

2.2 Modeling problem

The present study addresses the problem of quantitatively describing, up to PDE model kinetic and transport parameter uncertainty, the concentrations, temperature and flow state profiles of the syngas reactor startup and continuous operations on the basis of a low dimensional lumped model and one temperature measurement at the most sensitive stage, i.e., with the largest temperature slope change before the hotspot employed in industrial process control (Bashir et. al., 1992).

Our problem is solved with a two-step method: (i) first, the lumping set $\boldsymbol{\sigma}$ (5e) is manually adjusted to obtain a staged system with the least number of stages N_q and non-uniform spatial-partition $\boldsymbol{\zeta}_{nu}$ that quantitatively describes the continuous operation, and (ii) then, the resulting low dimensional model is restricted with the available temperature measurement (y), yielding an online N_q-SM of syngas reactor that described the startup transient.

The novelty of the present modeling approach in relation with our previous studies lies in the application of i) a procedure presented by Badillo-Hernandez et al. (2013) to design the lowest staged model with a lumping set $\boldsymbol{\sigma}$ of non-uniform spatial-partition in conjunction with a properly located temperature measurement of the efficient modeling criterion proposed in Badillo-Hernandez et al. (2017b), and ii) a criterion that establishes that the number of stages N_q must be chosen so that the discretization error (ε_{N_q}) of the N_q-SM with respect to its high-dimensional N_{pde}-SM counterpart is comparable to its modeling error ε_p in the light of its kinetics-transport parameter uncertainty ($\tilde{\boldsymbol{p}}$), i.e.:

$$\varepsilon_{N_q} \approx \varepsilon_p \tag{7}$$

The online modeling results will be put in perspective with previous related offline (Badillo-Hernandez et al. 2017b; Di Blasi and Branca, 2013) and online (Badillo-Hernandez et al. 2016, 2017a) modeling studies.

3. ONLINE MODELING

In this section, a low order online staged model for syngas reactor is designed in a two-part procedure: (i) the number N_q and the non-uniform spatial-partition $\boldsymbol{\zeta}_{nu}$ (or lumping set model $\boldsymbol{\sigma}_{nu}$ [5e]) are designed by means of a method proposed in Badillo-Hernandez et al. (2013) in conjunction with the quantitative criterion (7), and (ii) the replacement of the temperature state at measurement stage by the measured temperature yields a low dimensional online N_q-SM of (8) with better description capabilities than its offline counterpart.

3.1 Model lumping set

Here, the design of the lumping set $\boldsymbol{\sigma}_{nu}$ (5e) is addressed in order to obtain an offline N_q-SM, with the least number of stages N_q that describe the local behavior near the steady state of interest for the syngas reactor according to criterion (7), by means of a previously developed method (Badillo-Hernandez et al. 2013). For this purpose, the uniform and non-uniform spatial partitions $\boldsymbol{\zeta}$ are obtained and tested.

It is known that there is a body of standard schemes (Canuto et al., 1988) that generate a non-uniform spatial mesh partition $\boldsymbol{\zeta}_{nu}$ for a fixed N. However, the syngas reactors exhibit temperature and concentration spatial profiles with a very steep gradient that requires a specialized mesh distribution scheme. In consequence, the design of the spatial partition $\boldsymbol{\zeta}_{nu}$ for the offline lumping set $\boldsymbol{\sigma}_{nu}$ is performed on the basis of the steady state profiles of a high order N^+-SM according to the following summarized procedure (see details in Badillo-Hernandez et al. (2013)).

First, the spatial-partitions are set equal ($\Delta z_1 = \Delta z_2 = \cdots = \Delta z_N$) and the number of stages N^+ is increased until local steady-state behavior is described with certain modeling error ε_p (4). Then, on the basis of the resulting profile shapes, the number of stages N^+ is decreased and theirs spatial-partitions ($z_1, z_2, \ldots, z_{Nq}$) are adjusted heuristically to meet the modeling objective, regarding criterion (7), with the smallest number of stages.

The application of the above procedure yields: (i) a set of offline non-uniform spatial partition-based N-SMs with the least possible discretization error ε_N for every fixed N, and (ii) an offline N_q-SM (5) of non-uniform lumping set $\boldsymbol{\sigma}_{nu}$ with the least number of stages (N_q) that quantitatively describes the local dynamics near steady-state of interest according to error criterion (7).

3.2 On-line model

The second part of the proposed online modeling approach consists in substituting the heat balance equation of the i-th stage by the temperature measurement restriction equation

Table 2. Designed lumping sets and errors ε_N.

$\boldsymbol{\sigma}_u$		
N	$\boldsymbol{\zeta}_u[m]$	ε_N %
3	0.12 , 0.25 , 0.37	11.8
4	0.1 , 0.2 , 0.3 , 0.4	10
7*	0.06 , 0.12 , 0.18 , 0.25 , 0.31 , 0.38 , 0.44	7.8
$\boldsymbol{\sigma}_{nu}$		
N	$\boldsymbol{\zeta}_{nu}^{-}\,[m]$	ε_N^{-}
3	0.0 2, 0.06 , 0.23	10.5
4	0.016 , 0.04 , 0.09 , 0.30	9.2
5*	0.012 , 0.03 , 0.07 , 0.15,0.32	7.7
*: $N = N_q$		

$y(t) = \tau_i$ (5c) in the off-line staged model dynamics (5) with lumping set $\boldsymbol{\sigma}_{nu}$ obtained in the offline model procedure (Section 3.1), namely

$$\dot{\boldsymbol{x}}^* = \boldsymbol{f}(\boldsymbol{x}^*, \boldsymbol{u}, \boldsymbol{\sigma}_{nu}), \qquad \boldsymbol{x}^*(0) = \boldsymbol{x}_o^*, \qquad \boldsymbol{x}^*(t) \in X^*(t), \tag{8a}$$

$$\boldsymbol{\sigma}_{nu} = (N_q, \boldsymbol{\zeta}_{nu}) \tag{8b}$$

$$X^*(t) = \{\boldsymbol{x} \in \boldsymbol{R} | \boldsymbol{c}_y \boldsymbol{x} = y(t)\},\ \dim X^*(t) = n_x - 1 \tag{8c}$$

The resulting online model is an $(n_x - 1)$-dimensional (with $n_x = 3N_q$) non-autonomous dynamical system driven by the measurement signal y of the *actual* reactor dynamics (1f). Accordingly, the temperature of the closest element z_i of non-uniform spatial-partition $\boldsymbol{\zeta}_{nu}$ to the sensor location z_y (1f) is given by the sensor signal y with the possibility of improving the online SM description capabilities with respect to its offline version by virtue of the reactor information injection.

4. ONLINE MODEL FUNCTIONING

In this section, the proposed online modeling approach is applied to the pilot-scale syngas reactor (1). The functioning of the resulting low order online non-uniform N_q-SM is put in perspective with previous studies about offline (Badillo-Hernandez et al. 2013, 2017b) and online (Badillo-Hernandez et al. 2017a) uniform stages models.

In order to design the offline lumping set $\boldsymbol{\sigma}_{nu}$ the procedure of Section 3.1 is applied. First, a large number of stages $N^+ = 50$ (150 ODEs) and nominal parameters $\boldsymbol{p}$ are selected to obtain the reference solution $\overline{\pi^+}$. The modeling error ε_p (4) is computed disturbing four uncertain parameters (Amundson & Arri, 1978; Caram & Fuentes, 1982, Hobbs et al., 1992, Pérez et al.,2012) through an experimental factorial design of two levels (Raymond et al., 2009) on the N^+-SM. The set of

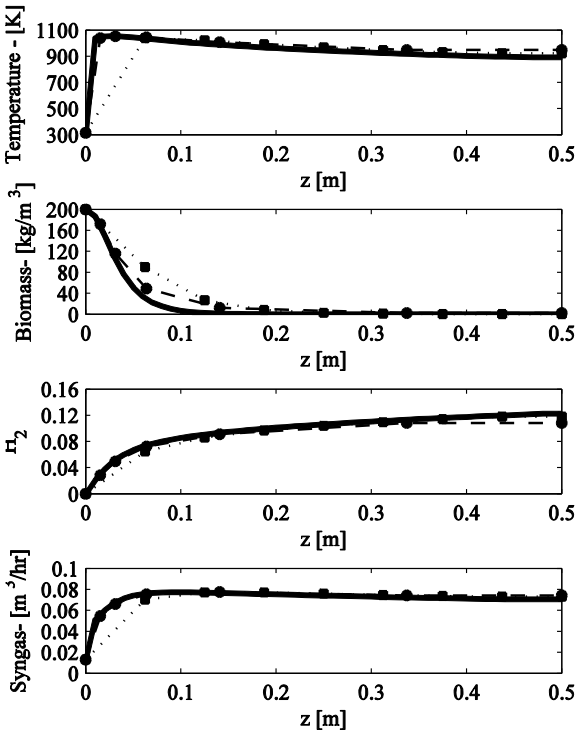

Fig. 2. Offline modeling of the continuous steady-state operation. Profiles for reference solution $\overline{\pi^+}$of $N^+ = 50$ (solid-line) and low order models of lumping sets $\boldsymbol{\sigma}_u^7$ (dotted-square line) and $\boldsymbol{\sigma}_a^4$ (dashed-circle line) for concentrations of components T, B, H_2 and gas flow q_g.

uncertain parameters produce a steady-state modeling error $\varepsilon_p \approx 8\%$, which is comparable with previous experimental studies (Manurung et al., 1993; Shwe, 2004). This set contains: i) the activation energy of biomass pyrolysis ($\pm 2\%$), ii) reaction enthalpy of char combustion ($\pm 5\%$), iii) heat diffusion coefficient ($\pm 5\%$) and iv) bed void fraction ($\pm 4\%$).

Secondly, the non-uniform mesh procedure is implemented for $N = \{3,4,5\}$ yielding the non-uniform spatial partitions $\boldsymbol{\zeta}_{nu}^{-}$ with the lowest approximation errors ε_N (6) of the non-uniform staged-models presented in Table 2. For our modeling purpose, the least number of stages of non-uniform spatial-partition is $N_q = 5$, since the set lumping $\boldsymbol{\sigma}_{nu}^5$ (15 ODEs) is sufficient to quantitatively (7) describe the ignition steady-state. For comparison purposes, a set of uniform spatial partition $\boldsymbol{\sigma}_u$ for N-SMs is included in Table 2.

Figure 2 shows the steady-state profiles of the reference solution $\overline{\pi^+}$ and the low order offline models of lumping set $\boldsymbol{\sigma}_u^7$ and $\boldsymbol{\sigma}_{nu}^5$. These results show that: (i) the high order ($N^+ = 50$) and the low order ($\boldsymbol{\sigma}_{nu}^5$ and $\boldsymbol{\sigma}_u^7$) models are equivalent descriptions in the sense of criterion (7), and (ii) the non-uniform spatial-partition $\boldsymbol{\zeta}_{nu}$ offers the lower stage numbers N than uniform ones to obtain the similar amount of error.

In order to describe the more complex startup operation with similar model dimension and errors to that obtained with offline models for the ignition steady-state description, a low order online staged model is obtained following Section 3.2.

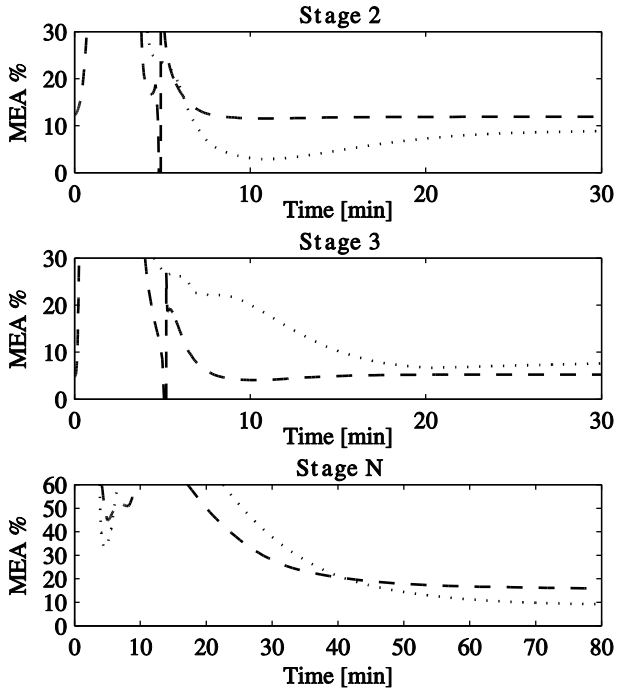

Fig. 3. Transient MAE of the online models in the startup operation for $\boldsymbol{\sigma}_u^7$ (dotted-line) and non-uniform $\boldsymbol{\sigma}_{nu}^5$ (dashed-line) structures in stages 2, 3 and N.

The offline dynamics (5) of structures $\boldsymbol{\sigma}_u^7$ and $\boldsymbol{\sigma}_{nu}^5$ are restricted by the temperature measurement located at the first stage ($y = \tau_1$) according to industrial criterion for tubular reactor control (Bashir et. al., 1992). Their functioning is illustrated in Figures 3 and 4 through the transient startup behavior of the overall mean absolute errors (MAE) at different stages, and effluent temperature, gas flow and concentrations of $H_2, CO, CO_2,$ and H_2O are plotted for the online N-SMs of non-uniform $\boldsymbol{\sigma}_{nu}^5$ and uniform $\boldsymbol{\sigma}_u^7$ lumping sets. The graphs show that better description capabilities (complex startup transient instead of only steady state) can be obtained with the same model dimension and error levels than its offline versions. Besides, the online model with non-uniform spatial-partition $\boldsymbol{\sigma}_{nu}^5$ provides a comparable performance with an estimated MAE of 5-12% than its

Table 3. Comparison of recent results of syngas reactor modeling studies.

Ref	Model Type	N (# ODEs)	Model Description
A	Offline	250-500 (3500-7000)	ISS
B	Offline	30 (90)	ISS
C	Online - GE	8 (23 + one sensor)	ISS & SO
D	Online	5 (14 + one sensor)	ISS & SO

A : Di Blasi (2000) GE : Geometric Estimator
B : Badillo et. al. (2017b) ISS : Ignition Steady State
C : Badillo et. al. (2016) SO : Startup Operation
D : Present study

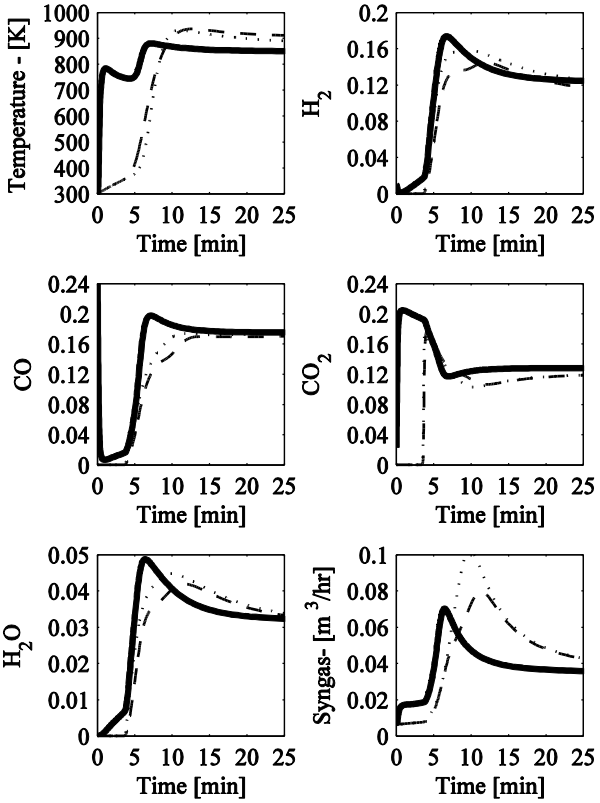

Fig. 4. Startup behavior with $N^+ = 50$ (solid-line) and low order models of lumping set $\boldsymbol{\sigma}_u^7$ (dotted line) and $\boldsymbol{\sigma}_{nu}^5$ (dashed line) for effluent values of $T, H_2, CO, CO_2, H_2O, q_g$.

counterpart $\boldsymbol{\sigma}_u^7$ of uniform partition, an order reduction of 28%, or, going from 50 down to 5 stages, we obtain a model reduction of 90%.

Finally, Table 3 presents a comparison of the proposed online non-uniform staged model with recent results of related syngas reactor modeling studies. In accordance, the online non-uniform 5-stage model has the same description capabilities and performance than the offline 30-stage model of Badillo-Hernandez et al. (2017b) and the online 8-stage geometric estimator of Badillo-Hernandez et al. (2016) with a significantly lower model dimension and simpler sensor data processing scheme. The most relevant improvement of the proposed approach is evidenced with the model reduction achieved by the 5-stage online model with respect to the large order (3500-7000 ODEs) offline models of PDE solvers (Di Blasi, 2000) commonly used in the field.

5. CONCLUSIONS

The problem of describing, up to PDE model kinetic and transport parameter uncertainty, the concentrations, temperature and flow state profiles of the syngas reactor startup and continuous operations has been solved with a low dimensional online model on the basis of an non-uniform mesh strategy and one temperature measurement.

The proposed online modeling approach is applied to a reactor case study showing that: i) the model with five non-uniform stages (15 ODEs) quantitatively describes the steady state and startup response with similar error to offline 250 (Di Blasi,

2000) and 30 (Badillo et al., 2017a) uniform stage models, ii) the lumping set scheme used reduces significantly the order of the model since five non-uniform stages have the same performance than seven (or eight for GE) uniform stages. The online staged model has the same form of the so called asymptotic observers (Dochain, 1992) or open-loop observers (Baratti et al., 1993), in the sense that the online measurement restricts the dynamics of a simplified model of the process without tuning gains of conventional innovation terms used in Kalman and Luenberger estimators.

This work is a point of departure to address problems about: i) to developed a systematic procedure to design the non-uniform spatial-partitions of the staged models, ii) the global description of the syngas reactor with online non-uniform staged models, similar to the study of Badillo-Hernandez et al. (2017b), iii) the limitations and capabilities of the online or offline modeling approaches regarding type (uniform or non-uniform mesh) of lumping set and iv) the robust detectability and controllability assessment of the syngas reactor online model with respect to sensor location and model dimension.

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