CHEMICAL ENGINEERING TRANSACTIONS
VOL. , 2023
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: Sauro Pierucci, Jiří Jaromír Klemeš

ISBN 978-88-95608-98-3; **ISSN** 2283-9216

Digital Twin of a tubular flow reactor oriented to the development of the control system

Riccardo Bacci di Capaci*, Simona Oliverio, Elisabetta Brunazzi, Chiara Galletti, Gabriele Pannocchia

Department of Civil and Industrial Engineering, University of Pisa, Largo Lucio Lazzarino 2, 56122, Pisa, Italy
riccardo.bacci@ing.unipi.it

This work is aimed at developing the first version of a digital twin of a plant prototype for the flexible production of different chemical formulates, to be used in various industrial fields, from the medical health to the tanning sector. The analyzed system is a tubular flow reactor characterized by multiple additions of components and by a series of static mixing elements. Firstly, the 1D dynamic modeling of the reactor is addressed, by defining the geometry, parameters, and operating conditions to reasonably describe the process evolution over time. Then, the corresponding feedback control system is designed to obtain the desired final products, by respecting the required specifications, in terms of mean concentration, degree of mixing, and flow rates. Different types of control architectures are derived and compared. The results show that not only SISO control schemes, but also multivariable solutions are possible, which effectively guarantee set-point tracking and disturbance rejection.

1. Introduction

The concept of Industry 4.0 is a core topic of global interest and is now leading to a major economic transformation; this technological paradigm pushes toward a totally automated production, and a digital and fully interconnected industry. Digital twin, that is, a highly complex virtual model, which intends to be the exact replica of its physical counterpart, as a machine, a plant, or a process, is one of the so-called Key Enabling Technologies (Wan et al., 2015).
The project Turboflux lays within the Industry 4.0 paradigms and aims at creating a highly flexible plant, to produce different chemical formulates, from the health sector, such as detergents, disinfectants, bactericides, but also substances typical of the tanning and paint industries. The desired formulations are produced from a limited number of basic components in liquid state, fed directly inline, and mixed by means of a series of static mixing devices installed within the pipeline (Thakur et al., 2003).
The Turboflux plant consists of two main sections: i) holds the static mixing system and the pneumatic pumps for the components and the formulate, and a buffer tank for temporary storing; ii) hosts the kegging machine for the final products and the control panels with external access in a safe area. The static mixing zone is comprised of a series of five parallel pipes connected by 180 ° curves (for around 20 m length in total): the main fluid is fed into the primary pipe; a series of smaller pipes is used for the additives. The main pipe is the mixing and reaction environment, and the final sector is a calm zone for stabilization, quality monitoring, and properties control. Components are fed with a dedicated pump, a control valve and two splitting valves, so they can be added in two different sectors of the pipe; mass flow meters are installed to guarantee a high precision in dosages. The recipes are developed for each final product; the relative quantitative and the procedure of injection are established in advance.
In this work, a first version of the digital twin of the Turboflux system is presented. The final version of this model will be then used for monitoring, diagnosis and controlling purposes, as well as to ensure safety and predictive analysis to counteract possible process perturbations (Bacci di Capaci et. al, 2017). The outline of the paper is as follows: Section 2 analyzes the system dynamics through mathematical models and numerical methods; in Section 3 open-loop analysis is performed, while in Section 4 different control system architectures are illustrated. Finally, conclusions are drawn in Section 5.

2. Methodology

The dynamics of a selected section of the Turboflux plant is investigated in this work and described by a simplified axial dispersion model. In reactors or mixers with tubular geometry, the axial dispersion is indeed a key phenomenon, which significantly influences the process dynamics and the main performance parameters, as yield and selectivity (Bahadori, 2012). In scenarios with a minimal geometric complexity, Computational Fluid Dynamics (CFD) offers various tools for an accurate investigation of the dispersion. To this aim, suitable CFD simulations, previously used for the computation of velocity and concentration fields of the system (Bacci di Capaci et al., 2022), are here exploited to estimate an average coefficient of axial dispersion, and thus to define the corresponding dynamic model.

Axial dispersion is a widely recognized approach for describing real flow conditions within a simplified model of a tubular reactor, that is, of plug flow (PF) type. As well-known, the PF model assumes that, for each axial coordinate, the fluid has a perfectly flat profile of any variables, as velocity and concentration. This means that no element of fluid overtakes or mixes up with any others, placed downstream or upstream the main flow direction. The axial dispersion model instead considers dispersive effects, such as slips and/or vortex formations; these stochastic phenomena are due to the local diffusion of components/reagents, which alters the perfect system segregation.

As basic relation, the following system of partial differential equations (PDE) is here adopted:

$$\frac{\partial < C_i >}{\partial t} = -\frac{\partial < u_z C_i >}{\partial z} + \frac{\partial D_{ax}}{\partial z}\frac{< \partial C_i >}{\partial z} + r_i \tag{1}$$

where $<u_z>$ is the average axial velocity through a general cross-section of the tubular reactor; $<C_i>$ is the average concentration of the *i-th* species on the same cross-section; D_{ax} is the axial dispersion coefficient; r_i is the reaction rate of the *i-th* species; z is the axial coordinate. Both concentration and axial velocity are functions of two independent variables, i.e., of space z and time t. With suitable assumptions (Moreau et al., 2017), Eq(1) can be reformulated as:

$$\frac{\partial < C_i >}{\partial t} + < u_z > \frac{\partial < C_i >}{\partial z} - D_{ax}\frac{\partial^2 < C_i >}{\partial z^2} - r_i = 0 \tag{2}$$

Note that the axial dispersion coefficient (D_{ax}) includes different contributions: molecular dispersion D_m, turbulent dispersion D_t, numerical dispersion D_n, and spatial dispersion D_s. This last contribution is at least one order of magnitude larger (10^{-2} m^2/s) than the others. Therefore, D_s can reasonably approximate the whole axial dispersion, both in laminar (Moreau et al., 2017) and turbulent regime (Talvy et al., 2007).

The main formulation produced within Turboflux plant is the well-known sanitizing gel, an alcohol-based mixture in aqueous solution. The World Health Organization provides the following composition: i) ethanol 80% v/v; ii) glycerol 1.45% v/v; iii) hydrogen peroxide 0.125% v/v; iv) distilled water to complement. For the sake of simplicity, the CFD simulations and the dynamic simulation of the preliminary digital twin assumed that the main (that is, vector) fluid flow rate is pure ethanol, and the additive fluid flow rate is single, comprised of pure distilled water. Therefore, in Eq(1) only one additive component is considered (i.e., $i = A$) and no reaction occurs ($r_A = 0$); that is, the tubular reactor reduces to an inline mixer. The profile of spatial dispersion coefficient $D_s(z)$ was obtained from the results of suitable preliminary CFD simulations performed in transient conditions, as suggested by Moreau et al. (2017). The following equation was thus adopted:

$$D_s(z) = \frac{< (u_z - < u_z(z) >)(C_A - < C_A >) >}{\frac{d < C_A >}{dz}} \approx D_{ax}(z) \tag{3}$$

where $<u_z>$ and $<C_A>$ are the mean velocity and concentration averaged over a selected cross-section; u_z and C_A are the local axial velocity and concentration, for each cell of the CFD discretization domain within the corresponding cross-section. Further details of the derivation of $D_s(z)$ are here avoided for the sake of brevity.

As a preliminary digital twin, the developed model refers to a limited subsection of the real plant. In particular, the simulation involves an initial empty pipe of 0.6 m length and a 2 m-length pipe equipped with static mixing devices of Ross LPD type (Ross, 2023). The following material and molar steady-state balances are considered:

$$\begin{gathered} Q_o^v \rho_0 + Q_A^v \rho_A = \dot{M}_{mix} \\ \frac{Q_A^v}{MW_A}\rho_A = \left(\frac{Q_A^v}{MW_A}\rho_A + \frac{Q_0^v}{MW_0}\rho_A\right) y_{A,in} \end{gathered} \tag{4}$$

where Q_0^v and Q_A^v are the inlet volumetric flow rate of vector and additive fluid, respectively; $\dot{M}_{mix}$ is the total mass flow rate after mixing; MW and ρ are molecular weight and density; $y_{A,in}$ is the molar fraction of additive fluid after mixing. The overall model consists of: i) a static summation node which represents a site of perfect

instant mixing, corresponding to the location of the additive fluid inlet; ii) a dynamic block, e.g., the value of inlet molar fraction ($y_{A,in}$) can be measured at the outlet ($y_{A,out}$) only after the block's dynamics. At each time instant, a mean axial fluid velocity is calculated, as $\bar{u}_z = \dot{M}_{mix}/(S\rho_{mix})$, where $S = \frac{\pi}{4}D^2$ is the constant cross-section of the pipeline, being *D* the diameter. The density (ρ_{mix}) of the considered ethanol-water mixture is evaluated by using a suitable correlation obtained in a previous study (Orsi et al., 2013), based on water mass fraction values. Note that the proposed approach can be easily extended to other sections of the real tubular mixer in future versions of the digital twin.

As known, an appropriate discretization method allows one to turn the initial PDEs problem into a system of ordinary differential equations (ODEs). Different algorithms have been developed within MATLAB for numerical integration of PDEs. The Method of Lines (MOL) is here adopted, as suggested by Pellegrino (2019). As ODE discretization method, the finite difference approach is here adopted. Eq(1) is thus reformulated in terms of y_A, i.e., the mole fraction of additive fluid:

$$\frac{\partial < y_A >}{\partial t} = - < u_z > \frac{\partial < y_A >}{\partial z} + \frac{\partial D_{ax}}{\partial z}\frac{\partial < y_A >}{\partial z} \tag{5}$$

where $C_A = C_T y_A$, being C_T the total molar concentration, which is constant. The first and second derivatives are respectively approximated by the first-order and second-order finite differences, both centered in z_k. Reformulating Eq(5), we get a set of *N* ODEs in the independent variable *t*, which can be easily integrated once defined the initial condition.

$$\frac{dy_A(z_k)}{dt} = -\bar{u}_z \frac{y_A(z_{k+1}) - y_A(z_{k-1})}{2\Delta z} + \bar{D}_{ax}\frac{y_A(z_{k-1}) - 2y_A(z_k) + y_A(z_{k+1})}{\Delta z^2} \tag{6}$$

with *k* = 1, … *N*-1. Note that, for the sake of simplicity, from the profile of $D_s(z)$ obtained with Eq(3), a mean axial dispersion coefficient is considered: $\bar{D}_{ax}$ = 0.04 m²/s. Given Eq(5), an initial condition (IC) with respect to time and two boundary conditions (BC) for the axial coordinate are to be imposed; in particular, as IC at *t* = 0, $y_A(0, z)$ = 0 ∀ *z* > 0; as BCs, at *z* = 0 $y_A = y_{A,in}$ ∀ *t* > 0, and at *z* = *L* (= 2.6 m) $\frac{dy_A}{dt} = 0$ ∀ *t* > 0. Ode45 function of MATLAB was finally used as numerical integration solver.

3. Open-loop Analysis

As first, a detailed analysis of the open-loop dynamics of the system modeled by Eq(6) is carried out. In particular, the effect of a generic variation of the mean input concentration is evaluated; afterwards, the system response to its actual inputs, i.e., the flow rate of two manipulated fluids (additive and vector), is investigated.

The propagation of the concentration of additive fluid is first evaluated by imposing an instantaneous variation of the mean input additive molar fraction ($y_{A,in}$); in particular, a step equal to 0.1. A constant axial velocity is imposed $\bar{u}_z$ = 6.89 m/s, for a total mass flow rate $\dot{M}_{mix}$ = 167.8 kg/min. Figure 1a shows the corresponding time response. Note that the system does not respond significantly for around 0.3 s; then, before reaching the new stationary value ($y_{A,out}$ = $y_{A,in}$), it presents some oscillations which decay in about 0.2 s. A brief parametric sensitivity analysis is also reported, by only varying the mean axial dispersion coefficient $\bar{D}_{ax}$; three other values are tested: 0.01, 0.05, and 0.08 m²/s. Figure 1b shows the corresponding responses. As the $\bar{D}_{ax}$ increases, overshoot and settling time decreases; that is, the input molar fraction of additive fluid (i.e., its concentration) appears at the outlet section more quickly and steadily; a higher coefficient indeed implies better diffusion of additive in the vector fluid, and then a more stable dynamic.

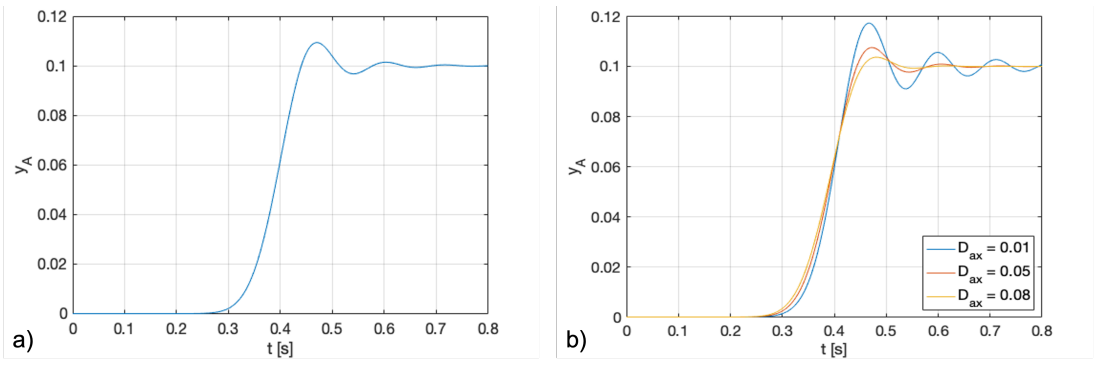

Figure 1: Propagation of additive concentration in the inline mixer: a) for nominal and b) different values of $\bar{D}_{ax}$

The trend of the mean molar fraction of additive in response to a step on the volumetric flow rate of additive fluid itself (Q_A^v) is then analyzed. As initial condition, a constant flow rate is assumed, 100% composed by vector fluid, that is, $y_A(0)$ = 0; a step of 10 L/min on Q_A^v is imposed. The specific flow rate values are then Q_o^v = 200 L/min and Q_A^v = 10 L/min. From molar balance on the additive fluid, the new stationary value of the mean molar fraction of additive is equal to $y_{A,out} = \frac{\frac{Q_A^v}{MW_A}\rho_A}{\left(\frac{Q_A^v}{MW_A}\rho_A + \frac{Q_0^v}{MW_0}\rho_A\right)}$ = 0.14. Figure 2a shows the corresponding system response. Again, the system does not respond for about 0.3 s; then, before reaching the stationary value, it presents oscillations decaying in about 0.2 s. This behavior recalls the underdamped dynamics of a linear system of the second order plus time delay (SOPTD), whose transfer function in Laplace domain is $P(s) = \frac{K_p}{\tau^2 s^2 + 2\xi\tau s + 1} e^{-\theta s}$.

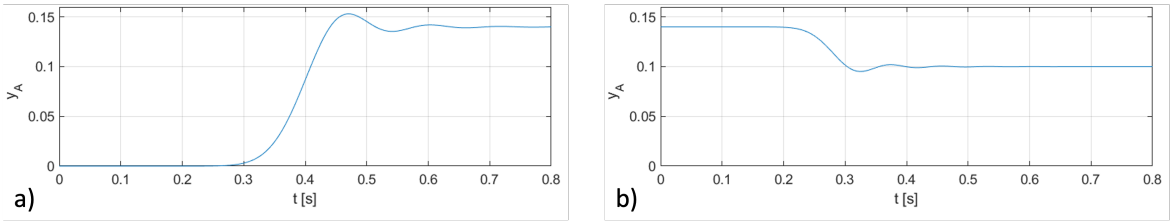

Figure 2: Propagation of additive molar fraction in response to step on: a) additive; b) vector fluid flow rate

To perform tuning of proportional-integral (PI) controllers for the digital twin, it was indeed decided to approximate the dynamics of the inline mixer with a SOPTD model. Hence, the four characteristic parameters are required: i) a time constant τ; ii) a time-delay θ; iii) a damping factor ξ. The fourth parameter, i.e., the gain K_p, can be easily obtained from the input(*u*)-output(*y*) stationary variations, i.e.: $K_p = \frac{\Delta y}{\Delta u} = \frac{y_\infty - y_0}{u_\infty - u_0} = \frac{y_{A,out}}{Q_A^v}$ = 0.014 min/L = 0.84 s/L. The three dynamic parameters are obtained by minimizing the error *e* between the response of the nonlinear system of Eq(6) and of the SOPTD model, in terms of IAE and ISE indices, defined as:

$$IAE = \sum_{j=0}^{N_t} |e_j| dt\,; \qquad ISE = \sum_{j=0}^{N_t} e_j{}^2 dt \tag{7}$$

where *j* is the time index and N_f is the final time sample. To this aim, a standard 3D grid-search method and an unconstrained optimization problem were performed; the optimal solution was indeed found by using *fminsearch* MATLAB function with the default options. Further details are here avoided for the sake of brevity; only final mean parameters are reported: τ = 0.037 s; θ = 0.33 s; ξ = 0.629.
Note that the controller tuning is done on the overall model *V·P*, comprised of two elements in series: the mixing system dynamics, i.e., the linear process model (*P*) just identified, and the control valve (*V*) dynamics, assumed as a first-order linear system: $V(s) = \frac{K_v}{\tau_v s + 1}$. Two valves are considered: i) the additive fluid valve V_A; ii) the vector fluid valve V_0. A constant time (τ_v) equal to 1 second is imposed for both valves. As for the gains, a linear relationship between the flow rate range and the percentage valve stroke is considered. The obtained values are 0.0033 L/s for V_A and 0.066 L/s for V_0. The root locus of model *V·P* is then investigated, and the basic technique of Ziegler-Nichols is adopted for tuning; obtained parameters are K_c = 768; τ_I = 3.86 s.
The same approach was followed for the relation between the vector fluid volumetric flow rate (Q_o^v) and the mean molar fraction of the additive fluid. Open-loop dynamics was studied (see Figure 2b), another SOPTD linear model was obtained (a negative gain K_p is now observed), and the corresponding PI controller tuning was performed. Details are here omitted for the sake of brevity.

4. Control systems

The different control architectures developed are here briefly illustrated. Basic controllers of traditional type are considered, i.e., with feedback structure and PI algorithm. In detail, 3 output variables are assumed measurable: 1) the mean outlet molar fraction of additive fluid (y_A), obtained by Eq(6); 2) the mixing degree (MD) at the axial coordinate *z* = 0.8 m; 3) the outlet total mass flow rate (M_{tot}). The output variables are assumed affected by white noise, a zero-mean signal with a fixed variance. Controlled variables are compared with the reference values (SP, Set-Point) and control errors are calculated, which then represent input variables to the control system. Once computed, control actions are then translated into the two manipulated variables, i.e., vector fluid (Q_0^v) and additive (Q_A^v) flow rates, whose ranges are 0-400 and 0-20 L/min, respectively. Note that MD was

previously evaluated from the results of extensive CFD simulations, as a function of *z*, for a volumetric flow rate of vector fluid equal to 200 L/min and for three different values of additive fluid flow rate, i.e., 1, 10 and 20 L/min. Figure 3 shows the profiles of the mixing degree obtained from postprocessing of CFD results. MD proves close to unitary for *z* > 1.6 m, that is, higher than the reference industrial value of 0.95, the so-called "perfect mixing", regardless the flow rate of additive fluid. As said, MD is controlled at *z* = 0.8 m, i.e., in a region of significant variability with respect to the volumetric flow rates ratio. To obtain a broader domain of solution for MD, a fitting surface was evaluated, that is, a non-linear static function of the type $MD = f(z, R^v)$, where $R^v = Q_A^v / Q_0^v$. In particular, the polynomial function *poly42* of MATLAB was employed, with a fitting coefficient R^2 = 97%.

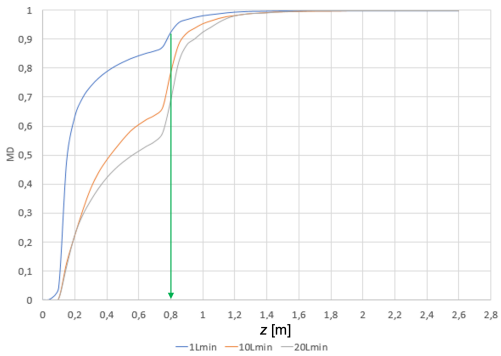

Figure 3: Postprocessing of CFD results: profile of the mixing degree for three levels of additive fluid flow rate

Several control architectures were then tested. As single SISO controllers, Type 1 controls the outlet mean mole fraction of additive (y_A), in case A) where the vector fluid flow rate (Q_0^v) is the only manipulated variable (MV), and in case B) where the additive fluid flow rate (Q_A^v) is the only MV; SISO Type 2 controls the mixing degree, in case A) with Q_0^v as single MV and B) with Q_A^v as MV. As decentralized MIMO architecture, in Pairing 1 y_A is matched with Q_A^v and M_{tot} is controlled with Q_0^v; Pairing 2 performs the opposite: y_A is matched with Q_0^v and M_{tot} is controlled with Q_A^v. As ratio controllers, Type1 is based on the set-point of mole fraction of additive (y_A^{SP}); Type 2, on the set-point of total mass flow rate (M_{tot}^{SP}). Only some architectures are briefly illustrated below.
In the SISO control scheme Type 1–B), the vector flow rate is fixed at its mean value of 200 L/min; the two parameters of the PI controller are suitably modified from the values shown in Section 3 to obtain improved responses. Proportional gain K_c must be positive to guarantee closed-loop stability, since the process has evident positive gain: when the flow rate of additive fluid increases, its mole fraction increases. Some step variations on the set-point, between 0.14 and 0.15, are imposed. The corresponding time trends of the mole fraction, mixing degree, and total mass flow rate are shown in Figure 4a. Figure 4b shows the time trend of additive flow rate, that is, the manipulated variable.

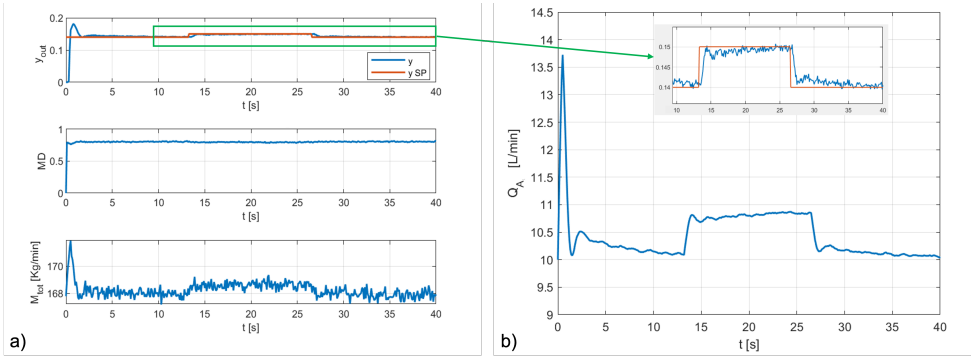

Figure 4: SISO control Type 1–B). Time trends of a) outputs and b) manipulated variable

Since the vector fluid flow rate is much greater than additive fluid flow rate, it is reasonable to manipulate Q_0^v to control the total mass flow rate. This happens in decentralized MIMO control Pairing 1, where parameters of two PI controllers are suitably retuned with respect to the corresponding SISO controllers to obtain improved responses by limiting loop interactions. Variations are imposed on two set-points at different times, to clearly observe the system behavior in terms of reference tracking and disturbance rejection. It is indeed possible to simultaneously guarantee the desired composition (y_A) and total mass flow rate (M_{tot}). Figure 5 shows the time

trends of the two controlled and manipulated variables. To move controlled variables to set-point, the vector fluid flow rate varies between 190 and 215 L/min; the additive flow rate, between 9.5 and 11.5 L/min.

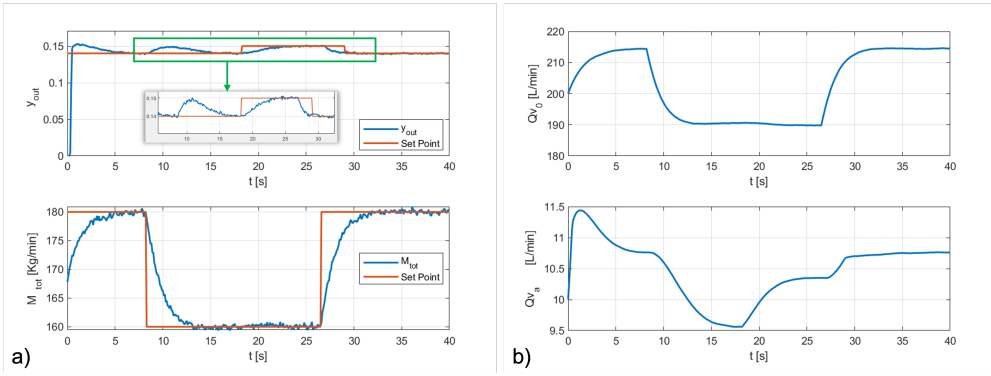

Figure 5: Decentralized MIMO control Pairing 1. Time trends of a) controlled and b) manipulated variables

Finally, in ratio control Type 2, the mean molar fraction of additive (y_A) is manipulated by the additive flow rate (Q_A^v) and, simultaneously, a desired flow rate of vector fluid ($Q_o^{v,SP}$) is imposed based on the set-point of total mass flow rate (M_{tot}^{SP}). In particular, the vector fluid flow rate is evaluated as $Q_o^{v,SP} = (M_{tot}^{SP} - Q_A^v \rho_A)/\rho_0$. Note that in this architecture, to ensure the appropriate flow rate ratio, it is also necessary to measure the volumetric flow rate of additive fluid Q_A^v. Results are here omitted for space limits.

5. Conclusions

In this paper, a first version of the digital twin of a tubular flow reactor was developed. The analyzed system is an inline mixer to produce the sanitizing gel, i.e., an ethanol-water mixture is considered. Firstly, the 1D dynamic modeling of the mixer is addressed; geometry, parameters, and operating conditions are defined to reasonably describe the process evolution over time. Among others, axial dispersion coefficient and mixing degree are evaluated from the post-processing of suitable CFD analysis. Then, different types of control architectures are designed to obtain the desired final products, by respecting the required specifications, in terms of mean molar fraction of additive fluid, mixing degree, and total mass flow rate. The results show that not only SISO control schemes, but also multivariable solutions are possible to guarantee set-point tracking and disturbance rejection.

Acknowledgments

This research was funded by the POR FESR project 2014–2020 ‘TURBOFLUX’ promoted by the Tuscany region.

References

Bacci di Capaci R., Scali C., 2017, Performance improvements of cascade and feed-forward control schemes for industrial processes, Chemical Engineering Transactions, 57, 985–990.

Bacci di Capaci R., Bellagotti F., Pannocchia G., Brunazzi E., Galletti C., 2022, A continuous flow reactor for the flexible production of different formulations: CFD-aided design, Can. J. Chem. Eng., 1-14

Bahadori A., 2012, Prediction of axial dispersion in plug-flow reactors using a simple method. Dispersion Science and Technology, 33, 200–205.

Moreau M., Di Miceli Raimondi N., Le Sauze N., Gourdona C., Cabassud M., 2017, A new numerical method for axial dispersion characterization in microreactors. Chem. Eng. Res. Des., 168, 178–188.

Orsi G., Roudgar M., Brunazzi E., Galletti C., Mauri R., 2013, Water-ethanol mixing in T-shaped microdevices. Chemical Engineering Science, 95, 174–183.

Pellegrino G., 2019, Numerical integration strategies of PFR dynamic models with axial dispersion and variable superficial velocity: the case of CO_2 capture by a solid sorbent. Heliyon, 5(9), 1–15.

Ross. Ross static mixers. https://www.staticmixers.com/, 12.02.2023.

Talvy S., Cockx A., Liné A., 2007, Modeling hydrodynamics of gas-liquid airlift reactor. AIChE Journal, 53(2), 335–353.

Thakur R. K., Vial C., Nigam K.D.P., Nauman E. B., Djelveh G., 2003, Static mixers in the process industries - A review, Chemical Engineering Research and Design, 81(7), 787–826.

Wan J., Cai H., Zhou K., 2015, Industrie 4.0: Enabling technologies. Proceedings of 2015 International Conference on Intelligent Computing and Internet of Things (ICIT 2015), IEEE, 135−140.