



# Semi-empirical modelling of the mass flow in a pilot-scale tubular reactor and tracking control

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## ABSTRACT

In this paper a model for a pilot-scale tubular reactor is developed using aggregated-parameters. The resulting model is a linear-varying system with time-varying delay. This model is simulated and compared to the results obtained from the experiments performed on the pilot-scale tubular reactor. In order to design a tracking control and considering the characteristics of the resulting model, predictive control techniques are used. The predictor is applied and a delay-free system is obtained. A tracking controller using the block control technique is proposed and is applied during simulation, the results are shown.

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## 1. Introduction

Mass flow in tubular reactors plays a significant role in the operation and performance of these devices (e.g. reactor yield). Mass flow is highly dependent on the geometry (i.e. design) of the reactor and of the helicoidal screw (if employed) as well as the mechanical properties of the material being transported. Flows are usually multiphase (i.e. solid–liquid–gas). Energy transfer and reaction phenomena usually occur along the reactor. Therefore, the mechanical properties of the material inside the reactor change respect to position and time.

Depending on the application, the dynamical models of tubular reactors for control purposes may span a wide range of mathematical complexity, from PDE if a detailed space-temporal description of state variables is needed (e.g. axial profiles of concentration in plug-flow reactors, [3]) to aggregated-parameters approximations (e.g. concentration values of glucose components at the end of a plug-flow reactor, [8]).

This work presents the construction of a semi-empirical model based on experimental data for the mass flow in a pilot-scale tubular reactor. The model describes accurately enough the dynamics of mass flow and avoid the complexity of PDE models. The approach used was a semi-empirical model construction via aggregated-

parameters, resulting in a linear-varying system with time-varying delay.

It is well-known that delays may dramatically limit the performance of the controllers and sometimes destabilize the closed-loop system [15]. This problem has been extensively studied and several controllers and stability criteria based on optimal control methods [22,17], including  $H_\infty$ , [6,9,11,5] and LMI's approaches [12], used Lyapunov–Krasovskii functional [16,18,2], have been proposed. Also, the linear-varying systems have been widely studied in [4,14].

The contributions of this paper are: **1.** The characterization of the mass flow dynamical behavior based on experimental data resulting in a linear-varying system with time-varying delay; this modeling of the mass transportation phenomena is important since the pilot scale tubular reactor in which the experiments are performed is a design that belongs to CINVESTAV ([20,21]), this means that there is no previous model for that reactor in the literature. **2.** The design of a robust tracking control that guarantees the mass flow to be constant in order to allow the latter application of chemical concentration models for the biomass.

The experimental rig is described in Section 2. Experimental data is provided as the basis for the dynamical model construction. In Section 3 the semi-empirical aggregated-parameters model is presented, as well as a comparison between this model and the experimental data. While in Section 3 the **Pressurization Section** of the reactor is modelled, in Section 4 the mathematical model is proposed for **Feeder Section** and both models are merged into one.

Having that model, considering the linear-varying system with time-varying delay, a predictive control is proposed in Section 5,

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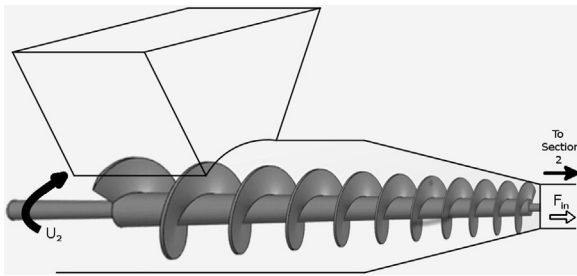


Fig. 1. Diagram of the feeder stage in the pilot-scale tubular reactor.

this controller is applied during simulation. Finally, the conclusions of this work are presented in Section 6.

## 2. Pilot-scale tubular reactor rig

The tubular reactor from CINVESTAV Guadalajara is used to make the pretreatment of biomass, as the first stage in bio-fuel production. The reactor is conformed by 3 parts or stages, and in each one the biomass (wheat straw), considered to be the Raw Material (RM) at the beginning of the process is put through a different treatment.

**Feeder Section.** Consists of an extruder conformed by a helicoidal screw inside a conic pipe. From a hopper, the RM is taken by the helicoidal screw driven by a motor. As the helicoidal screw moves the RM along the conic pipe the diameter of it decrements, causing the RM to compact until it forms a sort of cork, this cork enters as a flow of solid material  $F_{in}$  to the next section and prevents the pressure inside the reactor to escape. The RM is considered to be under mechanical treatment at this stage. A diagram of the feeder section is shown in Fig. 1.

**Pressurization Section.** This section is the reactor itself, consists of a tubular device with a helicoidal screw for conveying solid Extruded Material (EM) along the reactor under high pressure and temperature conditions. The EM is conveyed through the tubular reactor body at a  $F_{out}$  mass flow using the helicoidal screw rotating at  $u_1$  speed. This speed modifies the residence time of material inside the reactor, and depending on the desired characteristics of the treated material the speed  $u_1$  should be fixed (see [23]). The helicoidal screw cuts the EM entering the reactor, the volume of EM in each of the empty spaces in the reactor body is a function of  $F_{in}$  and  $u_1$  rates ratio. To avoid mass accumulation,  $F_{in}/u_1$  ratio must be less or equal to  $\beta$ , which depends on the reactor capacity. The high pressure and heat at this stage work as another treatment for the EM. A diagram of the pressurization stage is shown in Fig. 2.

**Output Section.** Consists of a valves system. In order to avoid the depressurization of the reactor, the pressurized material (PM) from the previous stage arrives to a chamber as a flow of solid material  $F_{out}$ , then the first valve is opened, causing the PM to enter a second chamber, after closing the first valve the second valve is opened and since the chamber is pressurized it causes a steam explosion that spews the PM, which is received in an output tray. This process discretizes the output mass flow  $F_{out}$  since the exploded material (XM) appears at the tray every certain time (after every explosion, every 4 min). The change of pressure and the explosion is the final treatment for the biomass.

## 3. Semi-empirical aggregated-parameters model for the pressurization stage

One of the experiments performed on the pilot-scale tubular reactor had the purpose of identifying the consequences of a change in the speed of the helicoidal screw, and how it is reflected on the

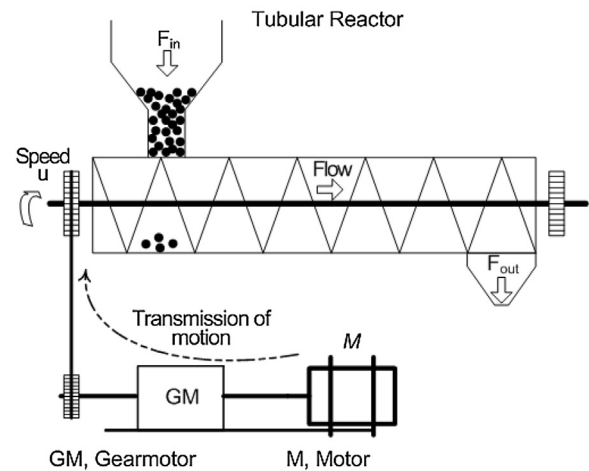


Fig. 2. Diagram of the pressurization stage in the pilot-scale tubular reactor.

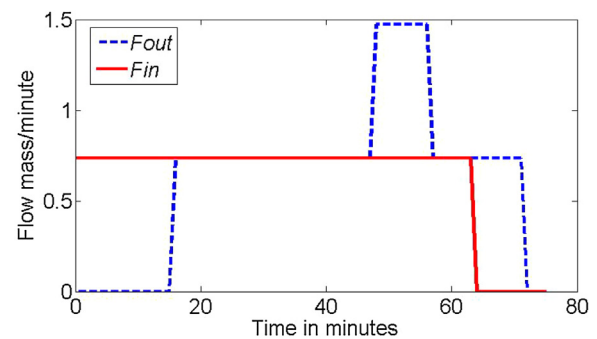


Fig. 3. Input and output flows.

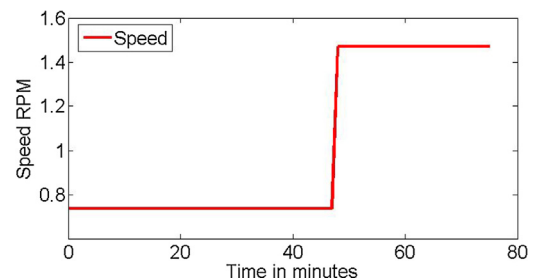


Fig. 4. Speed  $u_1$  of the helicoidal screw.

output flow, allowing to describe the dynamical behavior of the mass flow. The experiment was performed feeding by hand the pressurization stage, using compact solid units of material. For this experiment the material was not pressurized nor was submitted to high temperatures.

Figs. 3 and 4 show the mass flow and the screw speed trajectories of a typical experiment with a response to a step change in the screw speed  $u_1$ .  $F_{in}$  is fixed at 0.735 mass units per minute (MUPM). The screw speed  $u_1$  is 0.735 RPM. A transport delay of 16 min was observed. At  $t=49$  min,  $u_1$  was increased to 1.47 RPM. This was reflected immediately at the output flow, since it also increased to the double, 1.47 MUPM. This effect lasted 8 min. After this time, the flow returned to the steady state of 0.735 MUPM. At  $t=65$ , the mass feed ceased, the output flow continued for 8 more minutes and at  $t=73$  the output flow became zero. These events are summarized in Table 1.

The model for mass flow on a helicoidal screw has been proposed in other works, in [19] a model is presented, nevertheless

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