**A MODEL PREDICTIVE CONTROL FRAMEWORK FOR THE PRODUCTION OF SAFE AND FUNCTIONAL NANOMATERIALS**

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**ABSTRACT**

The increased production volumes of nanomaterials (NMs) and their various industrial applications have led to the need to develop advanced control methodologies that can address multiple objectives, related to the efficacy, functionality and safety of the produced NMs. The complexity of NM structures and additional requirements on achieving high yields and reducing possible adverse effects to humans and the environment, render the control of NM production processes a particularly challenging task. In this work we present a model predictive control (MPC) configuration for a series of plug flow reactors that synthesize Ag nanoparticles (NPs). In the first reactor the process of nucleation takes place and this is followed by autocatalytic growth in the second reactor. Three flows (solutions of silver nitrate, tannic acid and sodium citrate) are entering the first reactor and an additional stream of silver nitrate solution is added to the second reactor [1]. The manipulated variables are the flow rates of the 4 solutions, while their compositions are considered as disturbances. Different MPC problems are defined by specifying various control objectives.

The MPC methodology requires a process model to describe the dynamics of the system. To that end, Aspen DynamicsTM and in particular, the RPLUG model was used to develop a dynamic model of the two plug flow reactor process. Then, a neural network (NN) model was trained on a set of experimental data generated in the Aspen Plus Dynamics environment, using a series of step tests on the manipulated variables. Finally, the nonlinear NN model was linearised around the desired operational point. The produced linear model is used in the MPC configuration for the prediction of the future dynamic behavior of the process during the control horizon [2]. The performance of the MPC controller was tested and validated by its application on the original first-principles model of the process via integration of Matlab-Simulink® with Aspen Plus Dynamics. It is illustrated that the proposed methodology can lead to the design of functional control schemes that combine speed and robustness with low settling times and zero offset.

**KEYWORDS:** Safety by Process Control, Safety by Design, Nanomaterial Production, Model Predictive Control

**REFERENCES**

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