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"Dynamic Modelling of the INITIATE process"

Nicola Zecca[a]*, Vladimir Dikić[b], Eric van Dijk[b], Giampaolo Manzolini[a]

[a]Politecnico di Milano, Energy Department, Via Lambruschini, 4, 20156 Milan, Italy
[b]TNO, Westerduinweg 3, 1755 LE Petten, The Netherlands

Abstract

The climate crisis that the world is currently facing obliges the adoption of solutions to mitigate the emissions of greenhouse gas. The industrial sector represents a significant share of the total emissions of anthropic nature. The steel and the fertilizer industries are two of the most energy and carbon intensive, representing roughly 30% of all industrial CO_2 emissions [1]. Increase the energy efficiency, change the production process and integrate CCUS technologies are the main options to reduce the aforementioned greenhouse gas emissions. The INITIATE project aims to demonstrate a novel and symbiotic CO_2 utilization process that exploits the residual gases from the steel industry (i.e. BOFG and BFG) for urea production. The steel gases are first treated in the "Steel gas conditioning" section, in which the CO is converted into CO_2 and H_2 in a water gas shift reactor. The shift reaction is completed in the SEWGS multi-column system that simultaneously adsorbs the CO_2 and produces a N_2/H_2 stream. Operating the SEWGS technology in a PSA mode permits the continuous production of CO_2 and H_2/N_2 streams. The H_2/N_2 stream is then converted into NH_3 in the ammonia reactor before being eventually used for urea manufacturing with part of CO_2 captured by SEWGS.

The project combines both experimental work and theoretical modelling. The models are specifically useful to simulate the process at various scales, thereby enabling technical, economic and life-cycle assessments. One specific challenge that the project aims to address is the fluctuating composition of the residual steel gases. Conventional steady state modelling is not sufficient to capture the process effects on operations due to such fluctuations. Fluctuations in the feedstock composition causes potential deviations from the optimal temperature, throughput and product compositions, thereby affecting, economic and environmental performance. In order to understand how to optimally deal with the fluctuations, dynamic modelling is a powerful tool to design technical solutions that allows for flexible operations and mitigate the consequences of time variable feedstocks. The INITIATE project accordingly includes the creation of dynamic models for the simulations of transient behaviour to assess technology performance both at pilot and industrial scale.

In this paper the dynamic model of the INITIATE process and the optimisation of the (techno-economic) operation that deals with the BOFG dynamics are presented. As previously mentioned the INITIATE technology processes two residual steel gases, the BFG and BOFG. The BOFG is the one that exhibits the most significant time variations among these two. Different design choices are available to manage this variability. The key control parameter for the overall

* Corresponding author. *E-mail address:* nicola.zecca@polimi.it

process is the Hydrogen-Nitrogen ratio. This affects the production of ammonia and varies within the BOFG. The positive aspect on typical BOFG use is that the average ratio is closed to the stoichiometric value of 3. The aim of creating a dynamic model is to assess the performance of individual units and optimize the control strategy of the whole process to account for the dynamics and achieve the steady production of ammonia.
Temperature is particularly important as it depends on reactive feed composition. As the INITIATE process involves exothermic gas based reactions within tubular reactors, temperature control is crucial to maintain continuous, stable and safe operation, for instance to avoid hot spots. For all these reasons, the understanding of the thermal behaviour of the INITATE process with a variable feed composition is key to successful design and operation. Additionally, it is essential that product requirements are met with the optimal amount of utilities, feedstocks and inventory.
Generally, dynamic modelling can help to understand how product requirements and process temperature change with feed composition variations, and facilitate future analysis of process designs both at pilot and industrial scales. Specifically, this understanding is generated by mean of process modelling and simulation with AspenTech flowsheet simulation packages, namely Aspen Custom Modeler (ACM).

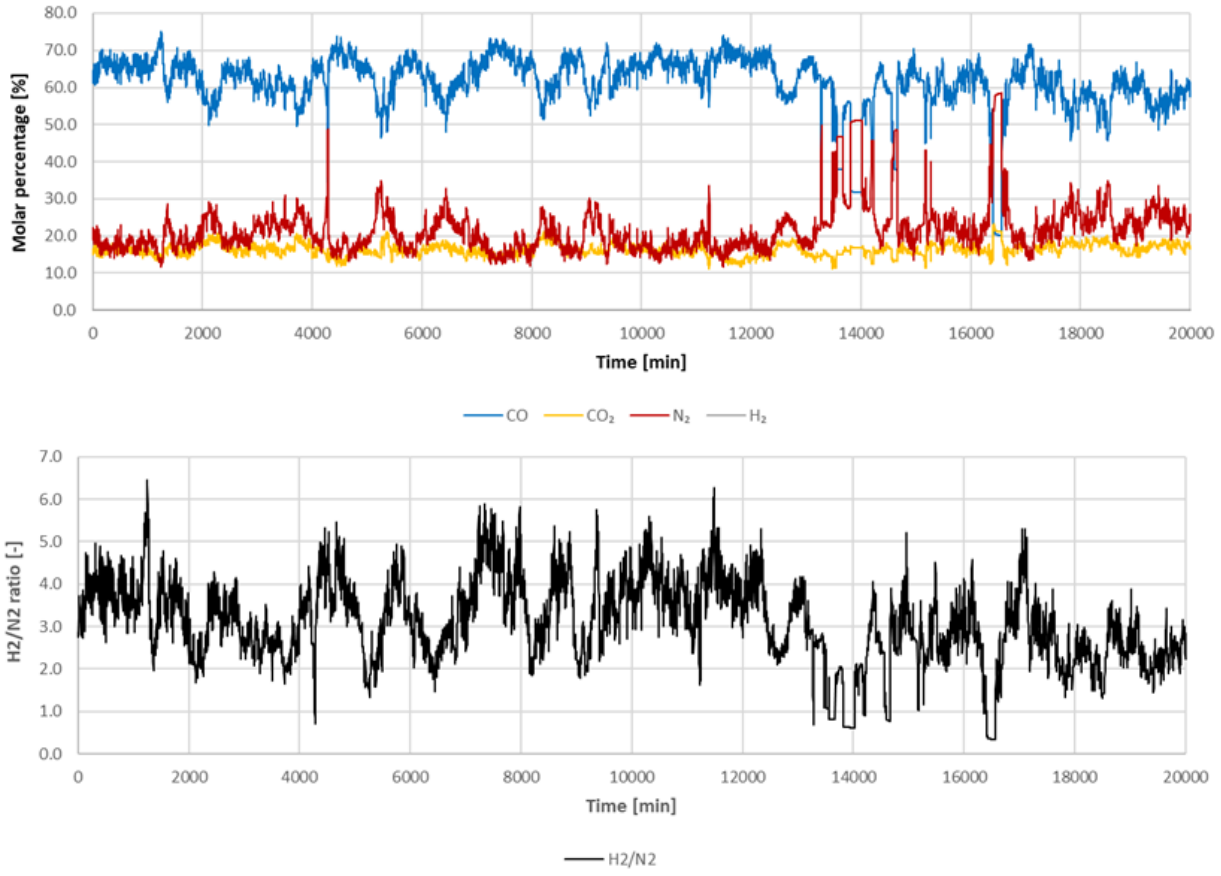

Figure 1: Example of simulated typical BOFG fluctuations composition and of H_2/N_2 ratio

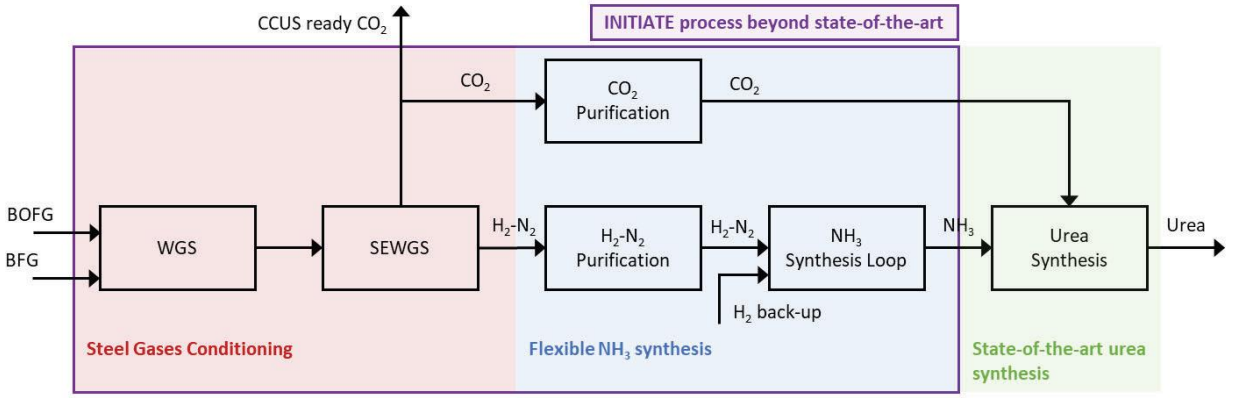

Figure 2: Block diagram of the INITIATE process

The four INITIATE reactive units that are required to convert residual steel gases to ammonia are modelled. These are i) the water-gas-shift (WGS), ii) the sorption-enhanced-water-was-shift (SEWGS), iii) the methanation and iv) the ammonia synthesis reactors.

Main assumptions of the WGS and Methanation reactor models:
- 1D Pseudo-homogenous Plug Flow Reactor Model
- Adiabatic operation
- Physical properties are calculated in time and space (Density, Heat Capacity, Viscosity…)
- Reaction enthalpy are calculated according to temperature change in time and space
- WGS intrinsic kinetics [2] are used while the catalyst activity factor was estimated using pilot data from the STEPWISE project. Estimation is performed at different reactor conditions using the estimation/optimization tool in ACM
- Methanation reaction kinetics are based on the methane-steam reforming kinetics from Lin & Liu, 2003 [3]

Main assumptions of the SEWGS reactor models:
- TNO's proprietary SEWGS Matlab model was used to generate the data that was used in System Identification analysis
- Resulting state-space models were implemented in ACM to describe the SEWGS's cyclic behaviour during the dynamic process simulation

Main assumptions of the ammonia reactor model:
- 1D Pseudo-homogenous Plug Flow Multi-Tubular Reactor Model
- Counter-current heat exchange between the cold gas (Tubes) and the pre-heated gas (Shell) is assumed. In addition adiabatic conditions are assumed
- Physical properties are calculated in time and space (Density, Heat Capacity, Viscosity…)
- Reaction enthalpy was calculated according to temperature change in time and space
- Reaction kinetics are based on the ammonia kinetics from Dyson and Simon 1968 [4]
- Estimation of catalyst activity is performed at different reactor conditions using the estimation/optimization tool in ACM

The dynamic model the plant is used to simulate the time-dependent behaviour of the processes within the plant and it can provide a wide range of results including (i) transient behaviour simulation, (ii) steady-state and dynamic stability analysis, (iii) optimization, (iv) process design and troubleshooting, (v) training and operator support, (vi) energy consumption analysis, (vii) environmental impact assessment. An example of the results from the simulations is shown in Figure 3.

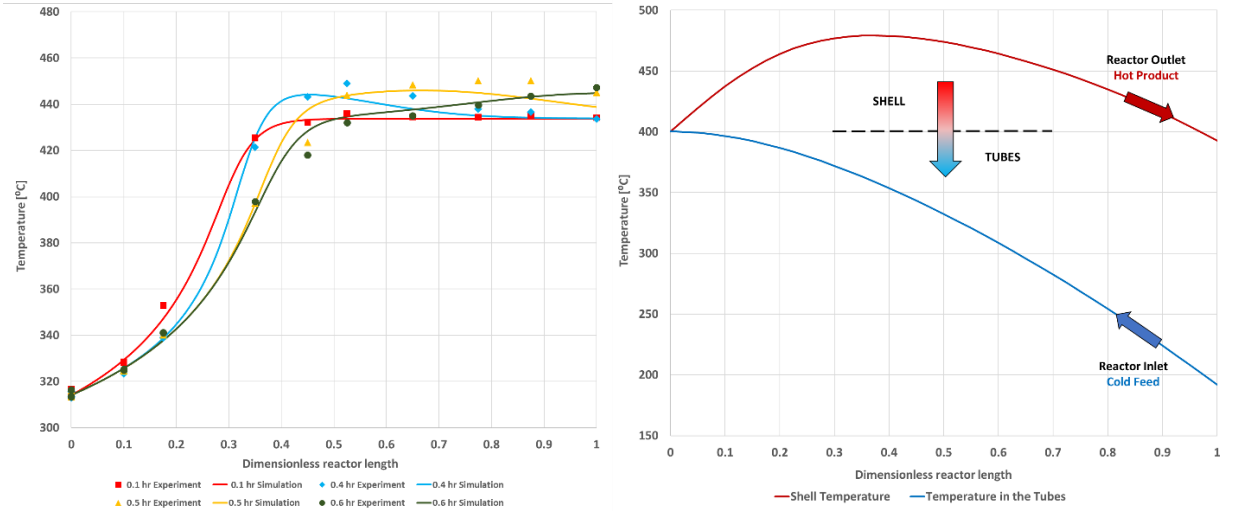

Figure 3: Temperature profiles 1) Dynamic response to the pressure change in the WGS reactor: Experiment vs Simulation, 2) Multi-tubular Ammonia reactor controlled operation

Keywords: Steel industry; Ammonia; Carbon capture and utilisation; SEWGS, Dynamic modelling; Controls

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