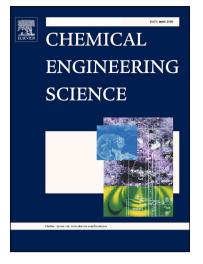
### Accepted Manuscript

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## ACCEPTED MANUSCRIPT

# Unsteady three-dimensional theoretical model and numerical simulation of a 120-kW chemical looping combustion pilot plant

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#### Abstract

In this paper, reactive unsteady three-dimensional numerical simulations of a chemical looping combustion (CLC) unit are presented. The configuration is a 120-kW pilot plant working with perovskite,  $CaMn_{0.9}Mg_{0.1}O_{3-\delta}$ , as the selected oxygen carrier. Numerical simulations were performed using NEPTUNE\_CFD code in the frame of an Euler-Euler approach by computing both gas and solid phases in an Eulerian technique, accounting for specific closures in order to model the interphase mass, and momentum and energy transfers. Heterogeneous reduction and oxidation (gas-solid) reactions were modeled by means of a grain model to account for the competing mechanisms of the chemical reaction onto the grain surface, the gaseous diffusion through the product layer around the grain, and the external transfer through the gas mixture surrounding the particle. Results from numerical simulations were assessed against experimental measurements and analyzed in order to acquire insight on the local behavior of reactive gas-particle flow in the CLC system. The theoretical/numerical tool developed in this work can be used for the design upgrade of crucial parts of the system in the stage of scaling-up from pilot to industrial plants.

Keywords: Chemical looping combustion, fluidized beds, gas-solid reactions, 3D CFD

#### 1. Introduction

Chemical looping combustion (CLC) is a process based on the combustion of fuel with the oxygen supplied by a solid material, called an oxygen carrier (OC). This technique, generally based on a dual circulation fluidized bed ([1]), involves the circulation of the oxygen carrier between two reactors: a fuel reactor (FR) for fuel combustion and an air reactor (AR) for OC regeneration. In the fuel reactor, a reduction reaction in solid OC by the gaseous fuel occurs, in which compositions can be expressed as  $MeO_x$  and  $C_nH_{2m}$ . The reduction reaction mainly produces  $CO_2$  and  $H_2O$  in the flue gas and converts the oxygen carrier to its reduced form,  $MeO_{x-1}$  (Eq. (1)). After the condensation of water vapor,  $CO_2$  is cooled and pressurized in stages to yield liquid  $CO_2$  ready for storage. According to the CLC operating mode, the reduced material ( $MeO_{x-1}$ ) is sent back to the air reactor and regenerated by air according to

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