Numerical simulation of fluids under high-pressure conditions

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1. INTRODUCTION

The suggestion to use supercritical fluids (SFs) is a century old, but the main progress in investigating and utilizing supercritical fluids has occurred mostly in the past 20 years [1]. They have been used (or proposed for use) as solvents, reaction media, processing media, and propellants. As example supercritical fluids can be effectively used in many industrial applications such as extractions (of vitamins, perfumes, etc.), syntheses, and processing steps. SFs are used to remove unwanted materials, such as caffeine and cholesterol from food products. They are also successfully used in many instances of analytical laboratory separations (extraction and chromatography). SFs are now replacing organic solvents in industrial processes. Indeed, many of these solvents have adverse environmental and health effects and supercritical CO_2 or water are attractive alternatives because they are inexpensive and offer minimal threat to both the environment and human health. SFs may be also found in the electronic industry where miniaturization efforts for the nanoscale technology recommend the use of fluids with zero-surface-tension property that are SFs. SFs are indeed becoming more essential nowadays.

Another domain of interest concerns propulsion with application to the automotive and aerospace science and technology where SFs may be considered as propellants [2]. Indeed, many fluid mechanical devices involve thermodynamic phase transition from a subcritical to a supercritical state. As example, the high-pressure combustion chambers of rocket engines operate at pressures and temperatures well above the thermodynamic critical points of the injected propellants, *i.e.* in a *supercritical* state (see Fig. 1). Such engines operate at very high pressure, typically of the order of 10.0 MPa whereas the critical pressure of hydrogen and oxygen is respectively 1.3 MPa and 5.0 MPa.

A final example concerns the *clean coal combustion and technology of transformation*. Indeed, coal, the most abundant energy resource, will continue to be dominant in China's energy scheme for a very long time [3]. Therefore, sustainable development requires the development and deployment of clean coal technologies such as supercritical and ultra-supercritical boilers, circulating fluidized bed combustion, and integrated gasification combined cycles. Clean Coal Technologies (CCTs) are technologies which facilitate the use of coal in a viable economic and human environment. A basic idea for the CCTs is the development of efficient systems in order to decrease the amount of coal used to generate the same amount of power. Some CCTs have already seen commercial application in industrialized countries. Advanced electric power generation systems that generate electricity

with greater efficiency and fewer environmental consequences are undergoing development in many countries.

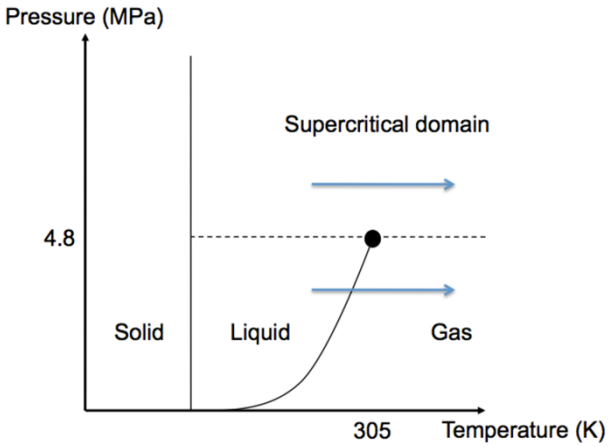

Figure 1: Pressure-Temperature diagram for ethane species.
Interest of the present study: arrows.

In particular, the pulverized coal combustion with supercritical steam cycles, together with flue gas cleaning units is under current research and development. However, units with subcritical boilers tend to have somewhat higher emissions of sulphur oxides (SOx) and nitroxides (NOx) per kWh than units with supercritical boilers. Indeed, subcritical systems are less efficient generating less kWh per unit of coal input. To improve the plant performance, the introduction of supercritical or ultra-supercritical steam conditions and the use of emission control devices is then necessary.

2. OBJECTIVES

Mixing is one of the most important phenomena in devices involving chemical decomposition because it determines the efficiency and stability of the chemistry along with heat transfer characteristics. In addition, most of the current understanding of turbulence and mixing is the result of atmospheric-pressure studies providing numerous numerical and experimental databases are available. A similar work has to be undertaken for sub-, trans- and super-critical flows investigation, *i.e.* real-gas effects have to be considered [4,5]. Indeed, this research field lacks of indisputable experimental data, useful for the numerical code validation. Simulation has made serious progress in the last decade but still need well-documented experimental test cases. Actually, only few experimental test-benches are able to reach/run supercritical configurations for propulsion applications, and among them, one test facility is located in Rouen at the CORIA Lab. (i.e. INSA de Rouen). It consists in an injection of ethane (C_2H_6) into nitrogen or helium at supercritical conditions (REFINE project). A database consisting of various values of spreading angle and breaking lengths has been realized for a range of pressure about [1-70] bar for a temperature evolving from 300K up to 500K. An example of such fluid injection is provided in Fig. 2: classical atomization processes (creation of drops for ex.) are replaced by a diffuse process. In chemical engineering, experimental data must still be highlighted.

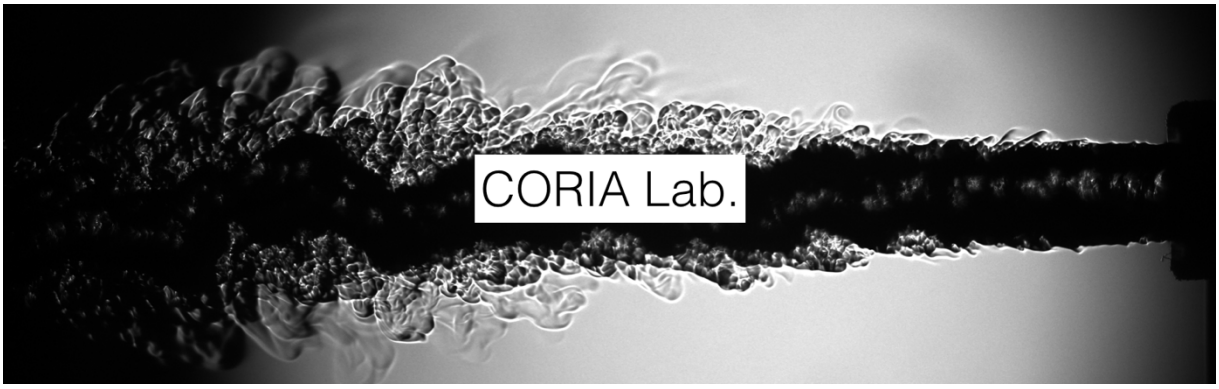

Figure 2: Injection of ethane into nitrogen at supercritical pressure.

The objective of the current project is the numerical simulation of fluid flowing under supercritical conditions. Such topic has already been addressed by classical formulations that use finite volume formulation for the description of the Navier-Stokes equations (through the numerical code SiTCom-B[1]), i.e. the balance equations describing the fluid dynamic. We already published several high-ranked papers [7-12] in which we deeply combined real-gas thermodynamic and high-pressure transport properties to an efficient solver of fluid dynamic. In the present study, it is proposed to address the same research topic, i.e. injection, mixing and chemical reaction under supercritical conditions, with a new fashion and promising numerical method: the Lattice Boltzmann Method (LBM). Interest in the lattice Boltzmann method has been steadily increasing since it grew out of lattice gas models in the late 1980s [13]. LBM is attractive because of its simplicity, its scalability on parallel computers, its extensibility, and the ease with which it can handle complex geometries. To assess the new strategy, a direct comparison with the classical approach (SiTCom-B) will be performed and the results from the REFINE project will be used. An open source code for the LBM will used. At least, two reference papers should be published.

Ph.D. Schedule:

Year 1: Bibliography. LBM code setup and simulation of simple low-pressure configurations. Derivation of equations for the modelling of supercritical conditions. Definition of injection and mixing test-cases.

Year 2: Validation of code programing and simulations of simple high-pressure non-reacting configurations. Simulation of a challenge to be define (bibliography). Integration of chemistry into the LBM code.

Year 3: Simulation of a challenge with kinetic decomposition. Comparison with literature (bibliography). Participation to scientific congress. Dissertation writing and Ph.D. Thesis defence.

[1] https://www.coria-cfd.fr/index.php/SiTCom-B

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