

SIMULATION OF NATURAL GAS FLUIDIZED BED USING COMPUTATIONAL FLUID DYNAMICS

Felix Severino de Farias Junior (UNICAMP)^{1,5}, Rubens Maciel Filho (UNICAMP)^{2,5}, Sergio Lucena (UFPE)^{3,6},
Jornandes Dias da Silva (UFPE)^{4,6}

¹ felix@feq.unicamp.br

² maciel@feq.unicamp.br

³ lucena@ufpe.br

⁴ jornandesdias@yahoo.com.br

⁵ State University of Campinas (UNICAMP), CP 6066, Campinas, CEP 13081-970, SP, Brazil, Phone: 55 + 19 + 3788-3971, Fax: 55 + 19 + 3788-3965

⁶ Federal University of Pernambuco (UFPE), Rua Prof^o. Artur de Sá, S/N,
Cidade Universitária, Recife, PE, Brazil, CEP 50670-090,
Phone: 55 + 81 + 3274-7274

The increasing availability of high performance and parallel computer environments has stimulated depth studies of complex reactor systems in chemical engineering. Using computational fluid dynamics approach, better description and comprehension of the most important phenomena taking place in the system can be accomplished, resulting in more efficient reactor and process design. Fluidized bed is a relevant system in many applications in process industries. Fluidized bed combustors are important alternatives to conventional ones, due to the fact that they promote large contact area between gas and solids and intense gas mixing throughout the bed, leading to cleaner burning and less pollutants emission, because the relatively low operating temperatures and isothermal profiles. In this work, computational fluid dynamics simulation of a natural gas fed fluidized bed was carried out. The simulated reactor bed was composed by inert particles (sand) with 350 μm . A two-stage kinetics model for methane combustion was used. Natural gas, the cleanest fossil fuel, was used in the simulated fluidized bed combustor, minimizing pollutant emissions even more. Dynamic simulations were developed with disturbances imposed into process input variables. The behavior of the simulated combustor was analyzed, and then compared to experimental data from literature.

CFD, natural gas, fluidized bed, fluid dynamics

1. INTRODUCTION

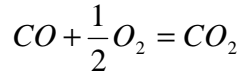
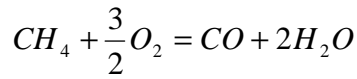
The increasing production and availability of natural gas in several parts of the world are creating better conditions and opportunities for the use and development of new technologies and applications for its consumption. Among the possible applications, it is detached the use of fluidized bed combustors in substitution to conventional ones. In the last years, a lot of research and investments have been made in this technology, due to the increase of the environment restrictions and constraints about the emission of pollutants and consequent need for cleaner alternative technologies.

Fluidized bed systems present interesting thermal properties for its application as combustors. The large contact area between gas and solids promotes high rates of energy generation during the solid fuel burning (Kuo, 1986) and very efficient thermal energy exchange between gas and solid particles. The Fluidized Bed Combustor (FBC) has diverse applications: generation of thermal energy, regeneration of catalysts, CO₂ production in large scale for other process feeding purposes, food processing, treatment of solid residues (drying, overhauling, calcination and incineration), among others. The adjustment of the flows of air and fuel gas allows the control of the working temperature in relatively low levels, 850-900°C (Pre et al, 1998). In such low temperatures, the emissions of NO_x are small, which represent an important advantage of the fluidized bed system over other conventional combustors. Natural gas is yet a relatively clean fuel when compared with common liquid fuels; in fact, it is the cleanest fossil fuel. The choice of natural gas as fuel in a fluidized bed combustor contributes even more for low formation of pollutants. With all these characteristics combined, the development of the technology of natural gas fluidized bed combustors assures great environment and economic importance.

In this work, a natural gas fluidized bed combustor simulation is carried out using computational fluid dynamics approach thought MFIX, a multiphase CFD code developed at the U.S. Department of Energy - National Energy Technology Laboratory (NETL) (Syamlal et al., 1993).

2. KINETIC MODEL

A natural gas combustion kinetic model can easily extend to more than 150 elementary equations. However, when simulating dynamics of combustors and reactors, a simpler mechanism approach is often desirable, because its much better computational performance. Considering a global two stage kinetic model, the methane combustion can be expressed by the following mechanism:



Dryer and Glassman (1973) considered a model of two stages for the oxidation of the methane in a reactor with turbulent flow and obtained the following kinetic rate expressions:

$$R_{CH_4} = 10^{13} e^{(-49600/RT)} [CH_4]^{0.7} [O_2]^{0.8} \quad (1)$$

$$R_{CO_2} = 10^{14.35} e^{(-45200/RT)} [CO][H_2O]^{0.5} [O_2]^{0.25} \quad (2)$$

This two stages model allows that the CO and CO₂ profiles along the bed be obtained, estimating the nonlinear behavior of the two steps global reaction.

3. CFD MODEL

A fluidized bed computational model was developed based on the fluidized bed described by Pre et al. (1998) using the Multiphase Flow with Interphase eXchanges (MFIx) code. The simulated reactor consisted of a 180mm diameter and 800mm pipe with a perforated plate distributor with 1.8% porosity (free area). Sand with 350 μm average diameter and 1400 kg/m³ specific mass was used as solid phase. A mesh grid of 18x50 points was considered for a 2D Cartesian coordinates simulation. Axial symmetry was considered. The bed was assumed to be isothermal and operating at 900 °C. Chemical reaction, momentum and mass balances were considered using the following general equations (Syamlal et al, 1993):

3.1 Momentum balances

Momentum balance for gas-phase:

$$\frac{\partial}{\partial t} (\epsilon_g \rho_g \vec{v}_g) + \nabla \cdot (\epsilon_g \rho_g \vec{v}_g \vec{v}_g) = \nabla \cdot \overline{\overline{S}}_g + \epsilon_g \rho_g \vec{g} - \sum_{m=1}^M \vec{I}_{gm} + \vec{f}_g \quad (3)$$

Momentum balance for solid-phase:

$$\frac{\partial}{\partial t} (\epsilon_{sm} \rho_{sm} \vec{v}_{sm}) + \nabla \cdot (\epsilon_{sm} \rho_{sm} \vec{v}_{sm} \vec{v}_{sm}) = \nabla \cdot \overline{\overline{S}}_{sm} + \epsilon_{sm} \rho_{sm} \vec{g} + \vec{I}_{gm} - \sum_{\substack{l=1 \\ l \neq m}}^M \vec{I}_{ml} \quad (4)$$

3.1 Mass balances

Continuity equation for the gas-phase:

$$\frac{\partial}{\partial t} (\epsilon_g \rho_g) + \nabla \cdot (\epsilon_g \rho_g \vec{v}_g) = \sum_{n=1}^{N_g} R_{gn} \quad (5)$$

Continuity equation for the solid-phase:

$$\frac{\partial}{\partial t}(\epsilon_{sm}\rho_{sm}) + \nabla \cdot (\epsilon_{sm}\rho_{sm}\vec{v}_{sm}) = \sum_{n=1}^{N_{sm}} R_{smn} \quad (6)$$

Species conservation equations (CH4, O2, CO, CO2, H2O, N2):

$$\frac{\partial}{\partial t}(\epsilon_g\rho_g X_{gn}) + \nabla \cdot (\epsilon_g\rho_g X_{gn}\vec{v}_g) = R_{gn} \quad (7)$$

$$\frac{\partial}{\partial t}(\epsilon_{sm}\rho_{sm} X_{smn}) + \nabla \cdot (\epsilon_{sm}\rho_{sm} X_{smn}\vec{v}_{sm}) = R_{smn} \quad (8)$$

The resulting partial differential equations system was solved through the finite volume technique. The convective flux discretization uses Superbee method and the iterative algorithm is a modified extension of SIMPLE (Syamlal, 1998).

4. RESULTS AND DISCUSSION

4.1 Simulation

The sand used as inert solid is recognized as a group B solid of Geldart classification. Under this condition, classical fluidization theory predicts 10cm diameter gas bubbles, fast ascending gas velocity in bubbles and a slower one in the emulsion phase. These characteristics were observed in the simulation results too, according to Figure 1. In Figure 1.a, a snapshot of bed void fraction distribution is represented. Figure 1.b shows an axial gas velocity profile with scalable gas velocity vectors, illustrating gas recirculation and dispersion phenomena. From Figure 1-b, it is possible to observe higher gas velocities in bubbles than in emulsion (larger vectors) and counter-current streams in the emulsion phase. This gas flow pattern promotes intense mixing and temperature homogenization along the dense phase of the bed, promoting an isothermal profile in a real bed.

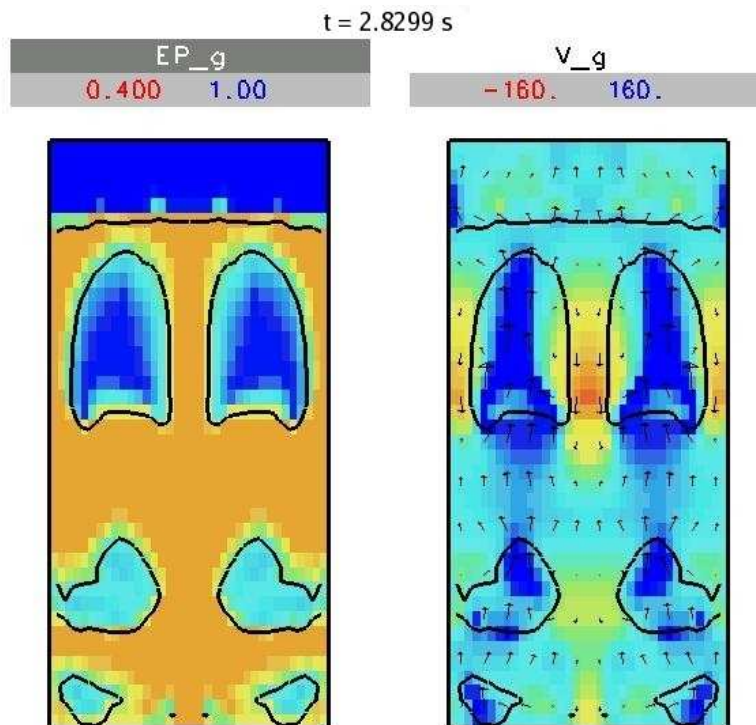


Figure 1 - a) Void Fraction profile

b) Axial gas velocity profile

In Figure 2, the dynamic oscillatory behavior of the fluidized bed for the carbon monoxide component after a step in methane feed is shown. The oscillation amplitudes are related to bubble sizes and positions and gas circulations patterns at each time sample.

4.2 Experimental Validation

Steady state simulation results were compared to data from literature (Pre et al., 1998). Average values of component molar fraction profile were calculated over a range of five seconds in dynamic simulation results and are compared to experimental data in Figure 3.

The results obtained by simulation presented faster methane kinetics at the entrance of the reactor. This can be attributed to the isothermal assumption of gas temperature along the reactor and to the limitations of the simplified kinetic mechanism adopted. Brien et al. (2003) point out that the present uncertainty in the kinetics law is a known source of errors in simulation of the combustion of the natural gas. It is expected that better results can be obtained with a better kinetic law and through a non isothermal simulation.

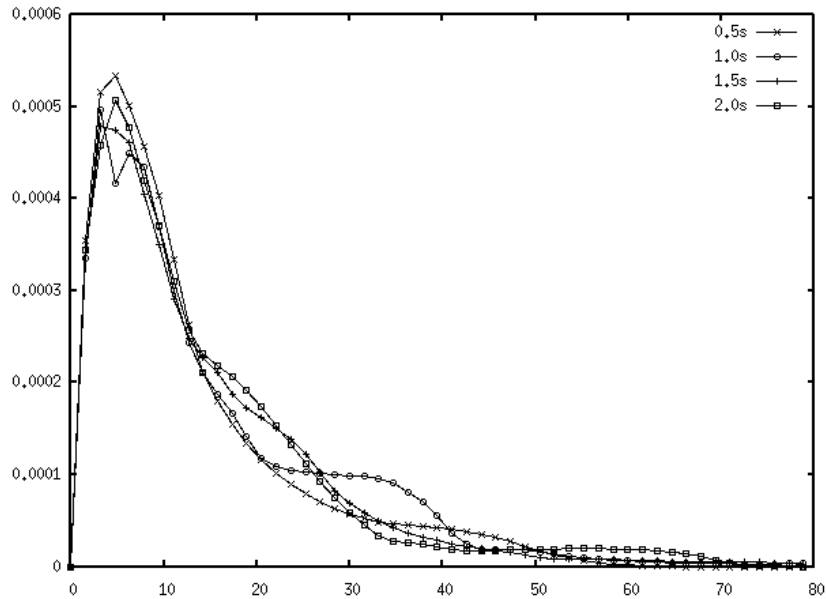


Figure 2 - Carbon Monoxide dynamic response profile after step in methane feed

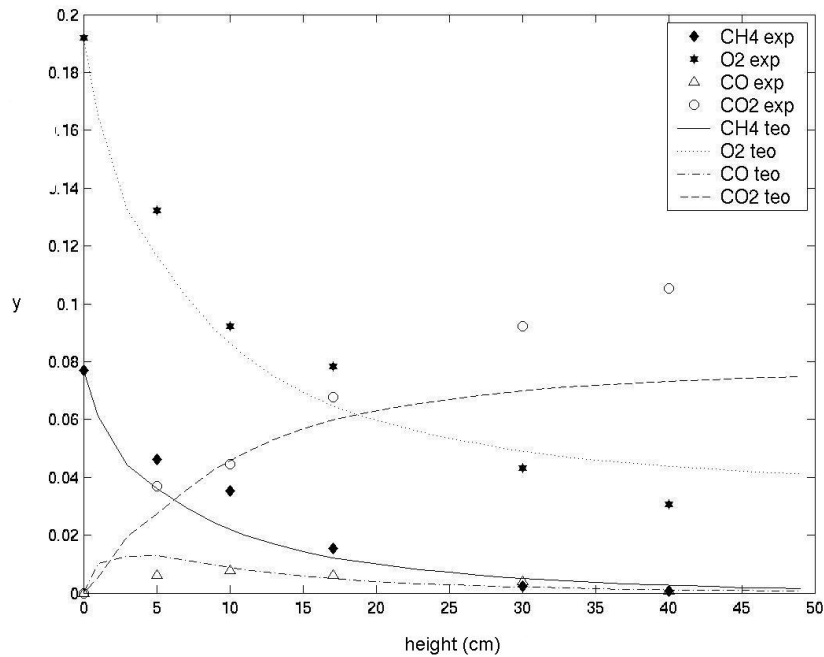


Figure 3 – Components molar fraction profiles

5. CONCLUSIONS

Despite of the simplifications assumed (isothermal bed, relatively small mesh grid and two stages methane combustion kinetics mechanism), simulation results were able to produce good predictions, both qualitatively and quantitatively for the fluidized bed. This shows the suitability of the proposed approach.

In this work, sand was used as inert particle which is a cheaper alternative to limestone. However, the limestone has an interesting property of sulfur adsorption that can be explored in future simulation works.

6. ACKNOWLEDGMENTS

The authors wish to thanks UFPE/ANP PRH-28 program, FINEP and PETROBRAS for the financial support.

7. REFERENCES

- DRYER, F.L.; WESTBROOK, C.K.; 1973. Chemical kinetic modeling of hydrocarbon combustion. *Prog. Energy Combust. Sci.*, 1984, Vol 10, pp 1-57. Pergamon Press Ltd.
- KUO, L.K. 1986. Principles of Combustion. 1 ed. New York, John Wiley & Sons, 601-614.
- MOUSTOUFI, N.; CUI, H.; CHAOUKI, J.; 2001. A comparasion of two- and single-phase models for fluidized-bed reactors. *Ind. Eng. Chem. Res.* 40:5526-5532.
- O'BRIEN, T. J.; SYAMLAL, M.; GUENTHER, C.; 2003. Computational fluid dynamic simulations of chemically reactive fluidized bed processes. **Third International Conference on CFD in the Minerals and Process Industries**. CSIRO, Melbourne, Australia. 469-474.
- PATANKAR, S.V. 1980. Numerical Heat Transfer and Fluid Flow. 1 ed. Series in Computational Methods in Mechanical and Thermal Sciences. Hemisphere Publishing Corporation.
- PRE, P.; HEMATI, M.; MARCHAND, B.; 1998. Study on natural gas combustion in fluidized beds: modelling and experimental validation. *Chemical Engineering Science*, 53:2871-2883.
- M. SYAMLAL, W. RODGERS, T.J. O'BRIEN, MFIK Documentation: Theory Guide, Technical Note, DOE/METC-94/1004, 1993.
- M. SYAMLAL, MFIK Documentation: Numerical Technique, Technical Report, DE-AC21-95MC31346, 1998.
- Multiphase Flow with Interphace Exchanges (MFIK). National Energy Technology Laboratory (NETL). U.S. Department of Energy. <http://www.mfix.org>