

MODELLING CO₂ CAPTURE BY CHEMICAL ABSORPTION

Paweł NIEGODAJEW, Dariusz ASENDRYCH, Stanisław DROBNIAK

Częstochowa University of Technology, Częstochowa, Poland

E-mail: niegodajew@imc.pcz.czest.pl, darek@imc.pcz.czest.pl, drobniak@imc.pcz.czest.pl

Key words: CO₂ capture and storage (CCS), chemical absorption, multiphase flow

Continuous growth of CO₂ emission is one of the most important threats of today's power industry. Among the methods currently being developed for carbon capture and storage (CCS) the post-combustion capture is the most preferred option. With this approach the flue gases are being sent through the absorber where CO₂ is separated by chemical absorption with the use of aqueous amine solution flowing countercurrently. Both phases pass through the packed bed where most of the chemical reaction occurs due to the enlarged contact area between phases.

The present paper reports on the numerical-experimental project aimed at building the CFD model of CO₂ capture process, the complex phenomenon including hydrodynamics of gas-liquid two-phase flow in porous region, chemical reaction and thermal effects due to its exothermic character. The model simulates the small-scale installation being ready for use. The Re values based on the gaseous phase inside the entire absorber decide about the laminar flow character.

The model was developed in ANSYS FLUENT as a 2D axi-symmetric and unsteady. The Eulerian/Eulerian approach was implemented to describe the two-phase countercurrent

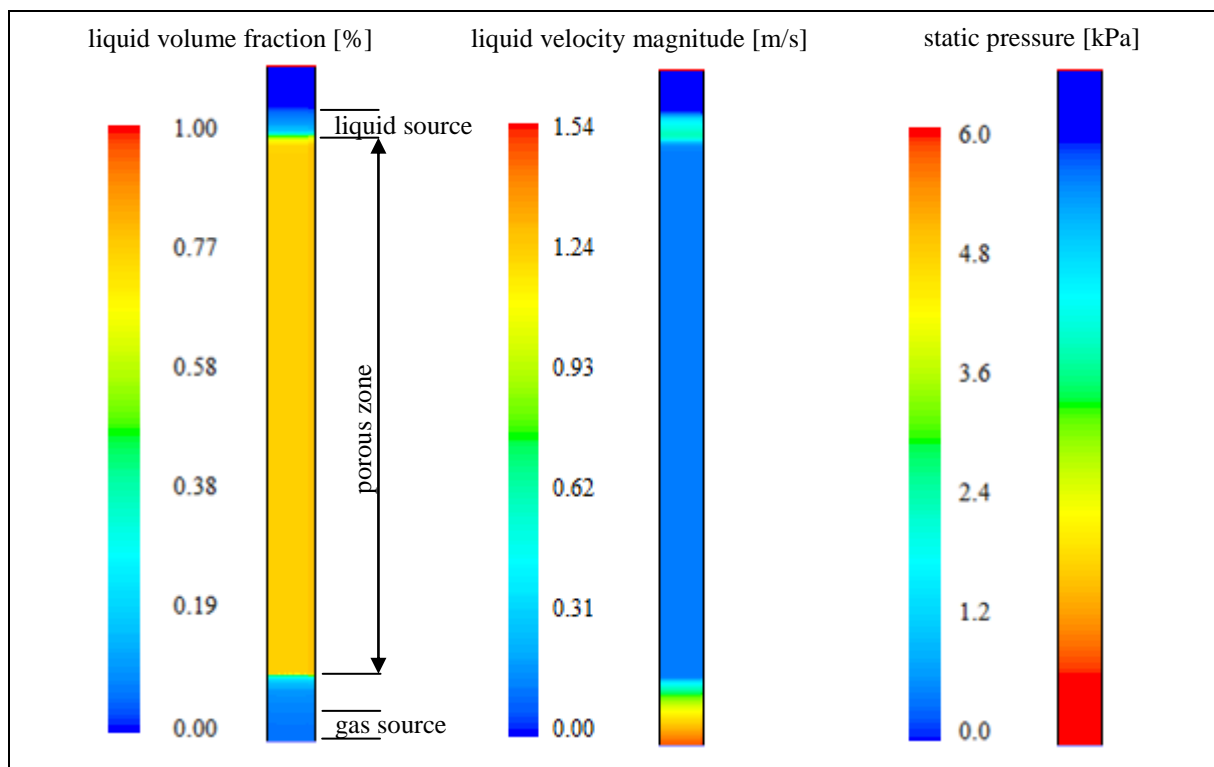


Fig. 1. Contour maps of liquid volume fraction (left), velocity magnitude (in the middle) and static pressure (right) inside the absorber column

flow with the phases interactions simulated by Naumann-Schiller formula. The porous region was modelled using the momentum sink described by the Darcy's inertial loss coefficients. The pressure inlet and outlet boundaries were chosen at the bottom and top of the column, respectively, to drive the flow and allow the phases to freely leave the domain. The gas phase enters the absorber column at its bottom, while the liquid is realised from the mass source located just above the porous region. These types of boundary conditions have been found as the most effective in terms of convergence of the solution (Xu et al., 2008).

As a first step the hydrodynamics of the 2-phase isothermal flow of non-reacting fluids has been studied. Water and air material properties were used as first approximation. Figure 1 shows some preliminary results of the flowfield in the form of contour maps. The distributions of three parameters are presented, i.e. volume fraction of liquid phase (on the left), velocity magnitude of liquid (in the middle) and static pressure (on the right). From the volume fraction (VF) distribution it is seen that the water is released from the source and enters the porous region (above the source water does not occur). Inside the porous region the VF is constant, while just below the liquid content dramatically drops down as a result of its acceleration due to the gravity force (see the velocity contour map). The static pressure distribution inside the domain shows clearly that the pressure drops only in porous region.

The model has been then extended by implementing exothermic reaction of chemical absorption of carbon dioxide by monoethanolamine (MEA), the most common amine sorbent for CCS purposes (Alie et al., 2005). The chemistry was modelled by laminar finite-rate model using Arrhenius expression to compute the chemical source term. According to Faramarzi et al., 2010 the chemistry of aqueous CO₂-MEA system may be approximated by a single-reaction mechanism of carbamate formation with negligence of the secondary routes (i.e. water ionization, hydrolysis and ionization of dissolved water, MEA protonation and others). The preliminary results of simulations have shown the physically sound behaviour of the system with CO₂ absorption rates at expected levels and satisfying temperature distribution in the absorber column. Further studies are, however, required to tune the model and verify its relevance for varying operating conditions. The special focus should be on chemistry of reacting media being the essential for the adequate modelling of CO₂ capture by chemical absorption.

Acknowledgements

The results presented in this paper were obtained from research work co-financed by the National Centre of Research and Development in the framework of Contract SP/E/1/67484/10 - Strategic Research Programme - Advanced technologies for energy generation: Development of a technology for highly efficient zero-emission coal-fired power units integrated with CO₂ capture.

References

- Alie C., Backham L., Croiset E., Douglas P.L. (2005): *Simulation of CO₂ Capture Using MEA Scrubbing: a Flowsheet Decomposition Method*, Energy Conversion & Management 46, pp. 475-487
- Faramarzi L., Kontogeorgis G.M., Michelsen M.L., Thomsen K., Stenby E.H. (2010): *Absorber Model for CO₂ Capture by Monoethanolamine*, Ind. Eng. Chem. Res., Vol. 49, pp. 3751-3759
- Xu Y., Paschke S., Repke J.-U., Yuan J., Wozny G. (2008): *Portraying the Countercurrent Flow on Packings by Three-Dimensional Computational Fluid Dynamics Simulations*, Chem. Eng. Technol. 31, No. 10, pp. 1445-1452