MULTI-SCALE MODELING OF THERMO-CHEMICAL PERFORMANCE OF AMMONIA CRACKING UNIT

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Ammonia Cracking Units (ACUs) play essential roles in mobile applications of fuel-cell technologies such as auxiliary electricity generating devices. Mathematical modeling of a practical ACU requires the coupling of geometric and fluid-mechanical aspects with chemical-kinetics complexity at unit and at system scale levels simultaneously.

The catalytic cracking of ammonia depends upon gas-phase and heterogeneous reaction mechanisms that can involve a number of chemical reactions. Direct chemistry coupling at different levels requires the significant extensions of the built-in capabilities of general-purpose Computational Fluid Dynamics (CFD) models. The latter should handle, in-parallel or simultaneously, the geometry of cracking units, peripheral devices, such as heat exchangers and their assembly configurations in a way similar to one shown in previous developments [1-3].

The present paper describes a novel capability to couple the full chemical kinetics with CFD and system-level analysis on the basis on the general-purpose CFD software, PHOENICS (http://www.cham.co.uk/phoenics.php). The approach exploits the structure of cracking units, in which the combined gas-phase and catalytic heterogeneous chemistry is confined within geometrically simple channels, and the engineering models of peripheral units.

Gas flow and catalytic combustion over the internal surfaces of the reaction zone walls are used to achieve thermal control. Hot combustion products from a fuel-cell purge/tail-gas exothermal oxidation taking place in combustion zone are used to support the endothermic ammonia cracking in the reaction zone. Figure 1 illustrates a typical configuration of such a unit.

The process and unit coupling is accomplished with the user-defined settings of INFORM capability available in PHOENICS (http://www.cham.co.uk/phoenics/d_polis/d_enc/in-form.htm). Fluid flow and heat- and mass transfer within the reaction and combustion zones are represented by CFD models that are developed to accommodate the appropriate chemical transformations. Coupling is made via the exchange of convective-radiation heat fluxes at the walls between zones. In addition to internal fluid flow, the customized PHOENICS model also represents immersed-solid heat transfer

within the reactor walls and heat- and mass exchange with external environment and with auxiliary equipment.

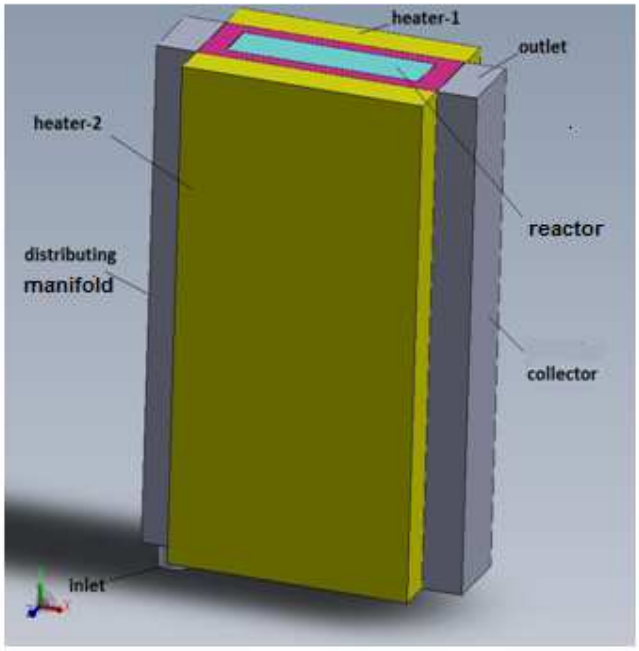

Figure 1. Illustration of ammonia cracking unit

Figure 2 illustrates a coupled solution for a particular ACU. The modeling results show the air oxidant path lines that are colored by particle variables. The path lines display a relatively complicated three-dimensional flow pattern. The hot products of purge-gas oxidation are cooled by heat transfer to the reaction zone in support of the endothermic reforming of ammonia. Heat transfer to the outer reactor walls also cools the combustion product flow.

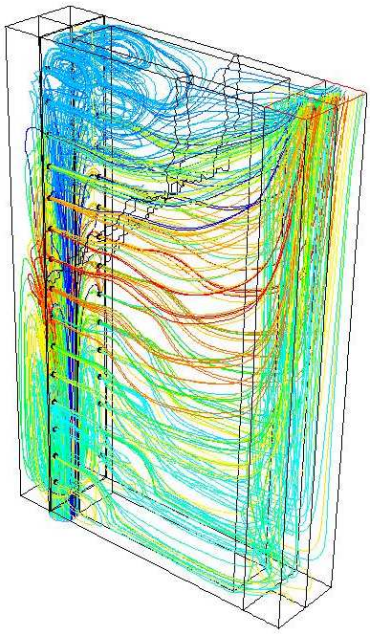

Figure 2. Path-lines in combustion zone colored by particle variables

A powerful CFD simulation capability couples complex gas mixture flow and heat- and mass transfer with highly nonlinear ammonia cracking and catalytic purge-gas combustion chemistry. Such a modeling tool plays by itself an important role in providing practical solutions of the unit/system design problems of ammonia cracking technologies.

The development of a CFD model for each equipment unit of an entirely coupled ammonia creaking system presents significant challenges. Creating the computational models and generating their numerical grids may take a long time and the total number of computational cells required may make the calculations impractical (i.e. the computations may take too long, if they can be done at all), and, if possible in principle, they could be very time-consuming and not suitable for design-time and run-time predictions. Therefore, a computational interface has been developed, within the main computational loop of CFD solver, for the thermo-chemical coupling links, which allow the system and heat exchanger network model of low scale to co-simulate with the higher-scale CFD simulations. By co-simulating a system model with CFD, the more realistic boundary conditions and component models are obtained economically, providing a deeper understanding of complex links in ammonia cracking systems.

A typical multi-scale modelling procedure uses ACUTE (Ammonia Cracking Unit's Thermo-Chemical Equations), a specifically developed PHOENICS-based system-level module, to model the entire assembly of ammonia cracking system including ACU and a network of supporting heat exchangers. The ACU itself can be modelled in detail using either fast-track lumped or more complex CFD technique (ACU2D or ACU3D), with the co-simulation to ensure that a two-way, bilateral exchange of inlet/outlet parameters between the ACUTE and CFD models provides a continuity of mass, heat and momentum transfers.

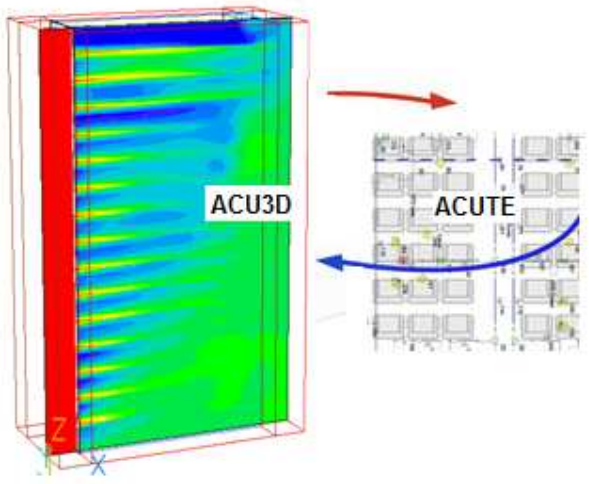

Figure 3. Coupled application of ACU3D and ACUTE models

Initially the co-simulation module attempts to procure a converged solution with the ACU3D/ACU2D model. Resultant boundary conditions and/or flow rates are exchanged, as shown

in Fig. 3, with the system-level ACUTE model so that it may update its solution, exchange and update the boundary conditions for the ACU3D/ACU2D model. There are two 'controls' that the user may use to influence overall convergence behaviour. These are the number of iterations of the ACU CFD solver before a data exchange of boundary conditions, and a relaxation factor which controls the extent of changes between successive calls to the ACUTE solver. When these parameters are appropriately specified, a converging iterative behaviour is generally obtained.

This paper provides an overview of the model that is under development by GenCell Ltd. in collaboration with ACFDA for computer predictions of technological behavior of ammonia cracking units. This is a system-level model with a co-simulation using CFD technique considering the thermo-chemical performance of all components that exchange mass and energy to produce the fuel-cell generator device's thermal and electrical output.

The models summarized in this paper are currently in use by GenCell. They indicate the correct performance trends and already have helped to explain a number of important observations both qualitatively and quantitatively. It is expected that testing and analysis of current implementations will lead to model refinements and enhancements. Furthermore, GenCell is carrying out a program of experimental work that will result in a set of comparative tests. Those will be used to further validate, calibrate and improve the models. The follow-up papers will report model details, enhancement and validation efforts as well as the simulation and observation results obtained, and technological effects achieved.

References

1. S.V.Zhubrin, Multi-Scale Modeling of Systems with Fuel Reforming, 2013, Available at https://dx.doi.org/10.13140/2.1.1909.0729
2. S.V.Zhubrin, Linking Detailed and Space-Averaged Models for Multi-Scale CFD Simulations, 2011, Available at https://dx.doi.org/10.13140/2.1.3940.6889
3. S.V.Zhubrin, Calculations of Thermal Performance of Heat Exchanger Loops, 2008, Available at https://dx.doi.org/10.13140/2.1.5178.0646