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CFD analysis of multi-phase turbulent flow in a solar reactor for emission-free generation of hydrogen

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Solar thermal cracking of natural gas is a promising process for hydrogen production because of its emission-free nature and yield of industrial grade carbon as byproduct. Solar reactors, where the two-phase solar thermochemical reaction takes place, are nearly experimentally inaccessible. Most instruments capable of measuring fluid flow cannot survive the harsh temperatures inside the reactor. As such, computational fluid dynamics (CFD) has been relied on to provide insight into the flow within the reactor. This paper presents the results of three dimensional CFD analysis of the solar reactor developed at Texas A&M University at Qatar by considering gas-particle transport with heat transfer, species transport and chemical kinetics using TAMU-Q supercomputing facilities. The results shows that a laminar flow shield on reactor walls and a vortex flow inside the reactor enhances the residence time and significantly reduces carbon deposition and clogging. The results also show that guide-vanes type of parallel carved channels on reactor walls creates better vortex.

Introduction

There have been studies dedicated to finding environmentally friendly solution to impending shortage of fossil fuels, but thermal decomposition of methane using concentrated solar energy has attracted researchers in recent years for its potential to lead to the development of CO_2 free hydrogen production process (Maag et al., 2009; Abanades et al., 2009; Muradov et al., 2009; Pregger et al., 2009; Kogan and Kogan, 2005; Dahl et al., 2004). The basic mechanism of the solar thermal cracking of methane, or “solar cracking” is simple: concentrated solar energy is directed to a reactor chamber, where natural gas is injected and absorbs solar energy resulting with hydrogen gas (H_2) and solid carbon (C) production. However, solar reactors, where the two-phase solar thermochemical reaction takes place, are nearly experimentally inaccessible. Because of that, most instruments capable of measuring fluid flow cannot survive the harsh temperatures inside the reactor. As such, computational fluid dynamics (CFD) has been relied on to provide insight into the flow within the reactor. Because of the size of the computing resources necessary to properly account for all of the physical mechanisms within the solar reactor, the current state of numerical simulations only provide a

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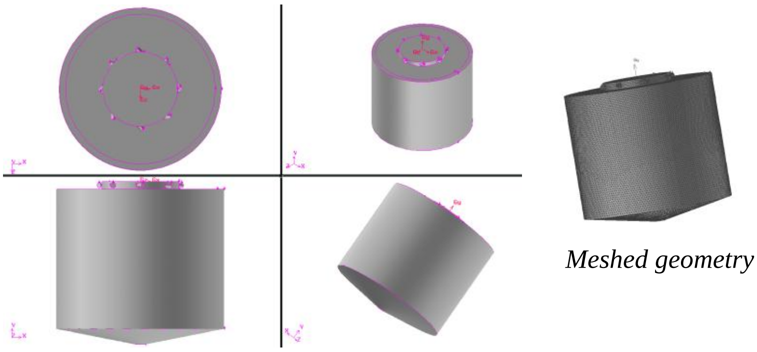
limited level of insight. In order to include radiation, particulate flows, and a high level of turbulence modeling, vast amounts of computing resources are needed. This requires the CFD algorithm to be capable of: (i) utilizing supercomputing facility with enhancement in memory, (ii) multi-physics capabilities including radiation and particulates, and (iii) advanced turbulence modeling. CFD simulations can provide an insight of the temperature distribution and flow characteristics inside a solar reactor. That information can be used to enhance reactor design and efficiency. The two-phase, three-dimensional CFD model we have developed includes kinetics, heat transfer and incoming solar flux for our solar reactor, which we named “aero-shielded solar cyclone reactor.” The validation to our CFD model has been carried out against the experimental results of Kogan group of Weizmann Institute of Science (Kogan et al., 2004) and Steinfeld group of Swiss Federal Institute of Technology (Hirsch and Steinfeld, 2004a; Hirsch and Steinfeld, 2004b), where the details of the validations can be found in Ozalp and Kanjirakat (2010), and Ozalp and Jayakrishna (2010). This paper presents the most recent results of our CFD analysis used in the improvement of our solar reactor design and presents the latest reactor concept.

Main issues with solar cracking reactors

There are two main issues affecting the performance of solar cracking reactors: carbon deposition, and change in incoming solar flux due to change in weather conditions. The first problem occurs from carbon accumulation on reactor window, walls and exit. Once the carbon particles accumulate on reactor window, incoming rays cannot fully penetrate through the window. This reduces the temperature inside the reactor and lowers the methane to hydrogen conversion efficiency. Carbon deposition at reactor exit is the biggest problem of solar cracking reactors, which ends up with reactor clogging. The second major problem that solar cracking reactors having is the change in radiation flux due to change in weather conditions, e.g. high flux when the sky is clear, low flux when there are clouds, rain, dust storm etc. This problem is actually shared by all solar thermal reactors and affecting their performance because it is not possible to have quasi equilibrium condition and/or semi-constant temperature inside the reactor when the solar flux keeps changing due to the changes in weather. This paper focuses on the carbon deposition problem and provides our method to track and solve this problem.

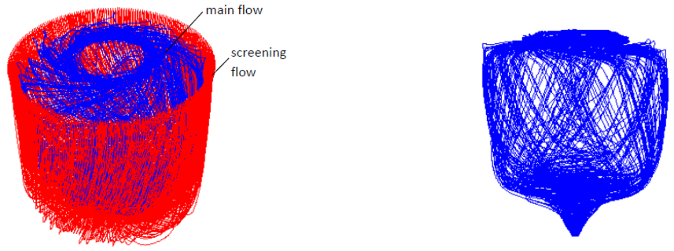


Meshed geometry

Figure 1 Aero-shielded solar cyclone reactor

CFD simulation of the aero-shielded solar cyclone reactor

In order to understand the flow behavior and track the carbon particles inside the reactor, we have applied our validated CFD model to our aero-shielded reactor concept. The three-dimensional geometry for simulations is built using GAMBIT, which is also used for generating the non-uniform unstructured grid in the geometry. The basic geometry with flow conditions and the adapted grid used for simulations are shown in Figure 1. In this concept, natural gas main flow is injected through impeller disk jets from the top center of the reactor with a 45° angle at a flow rate of 7m/s making a strong vortex concentrated in the middle of the reactor. Our numerical model includes RNG k-ε turbulence model, discrete ordinate radiation model, species transport with volumetric reactions, discrete phase model for particle, finite volume method – SIMPLE algorithm, and convective formulation – second order upwinding. The details of our numerical methodology can be found in Ozalp and Jayakrishna (2010). Our CFD simulation tracked carbon particles via Lagrangian particle tracking and we optimized the reactor configuration until we achieved a laminar flow shield on the walls and a vortex flow inside are obtained. Figure 2 shows the isometric and top view of this laminar and vortex flow inside the aero-shielded solar cyclone reactor. As it is seen, laminar flow and vortex flow are very close (2 cm apart) but do not disturb each other. This flow formation provides several advantages: First, laminar flow shield constantly sweeps the walls with a flow rate that is powerful enough to not to let carbon particles deposit on reactor walls. Secondly, vortex flow keeps carbon particles inside the turbulence, which reduces the number of carbon particles moving towards the walls. Another advantage of the vortex flow is it enhances the residence time. This way, carbon particles stay inside the reactor longer and continue serving as a radiation absorber and nuclei for reactions yielding more methane to hydrogen conversion. Finally, vortex flow prevents carbon particles from moving to the exit altogether at a time so that they do not accumulate at the exit causing clogging.



Isometric view

Main flow – Front view

Top view

Screening flow – Front view

Figure 2 Pathlines colored by surface ID

Front view of the main flow shows how methane flow forms a vortex inside the reactor. On the other hand, the screening flow maintains a laminar shield not letting carbon particles stick on the walls. We have tested several screening flows -such as helium, hydrogen, nitrogen- and found out that argon serves as the best wall screening gas. On the other hand, our simulations showed that to keep carbon particles away from the reactor window, hydrogen serves as the best window screening gas. Although we have achieved what we were looking for with this flow configuration, we continued our research to see if we can obtain a better vortex. Our research results showed that by changing the inlet flow rates, angles, location, velocity etc., it is not possible to have a better vortex than shown in Figure 2 for this particular reactor geometry. Since our earlier study published in Ozalp and Jayakrishna (2010) on the validation of Steinfeld group’s solar reactor showed us that helical carving on reactor walls can improve the overall reactor efficiency, we tried a different type of wall carving to see if that would make any difference. Next section presents the results of that research interestingly showing that guide vane type of parallel carving on reactor walls indeed create a better vortex.

CFD simulation of the aero-shielded solar cyclone reactor with parallel guide vanes

It was shown by Steinfeld group’s experiments that helical carving on reactor wall shown in Figure 3 increases solar reactor performance (Hirsch and Steinfeld, 2004a; Hirsch and Steinfeld, 2004b; Trommer et al., 2004). This design provides higher temperatures due to more efficient radiation absorption at the reaction site with this vortex flow, which is created by methane flowing through the helical carving, e.g. creating N-plug flow instead of plug flow.

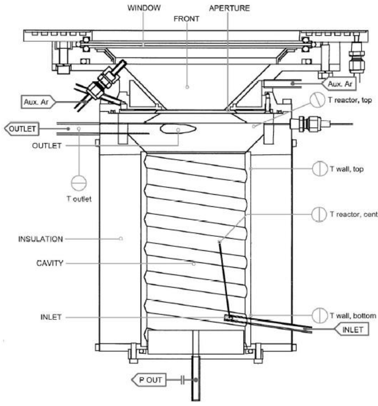


Figure 3 Scheme of Steinfeld group’s reactor configuration (Trommer et al., 2004)

Our numerical analysis successfully predicted their published experimental results, which helped us to understand the physics behind the effects of helical carving design (Ozalp and Jayakrishna, 2010). Figure 4(a) and 4(b) show our normal and meshed 3D geometry to simulate Steinfeld group’s reactor of Figure 3. As the next step, we have developed a reactor concept with carving different than Steinfeld’s group reactor. In our design, we put channel type of parallel guide vanes on reactor walls to direct the wall screening flow, and then applied our successful code to this concept to see the effect of guide vane type of parallel carving on the flow field. In this reactor concept, the laminar flow sweeping the walls has 0.5 cm thickness and it is injected from the manifold located at the top of the reactor. The flow is guided through channel like vanes of 0.5 cm depth. Figure 5 shows the simulation result of the aero-shielded solar cyclone reactor with guide vanes.

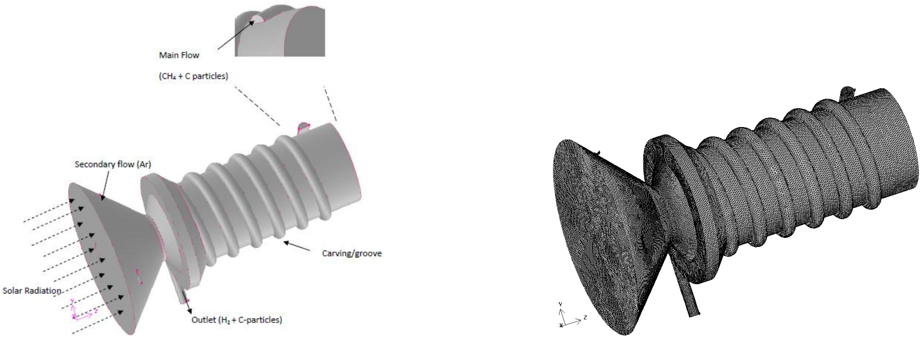


Figure 4 (a) Reactor geometry *(b) Meshed geometry*

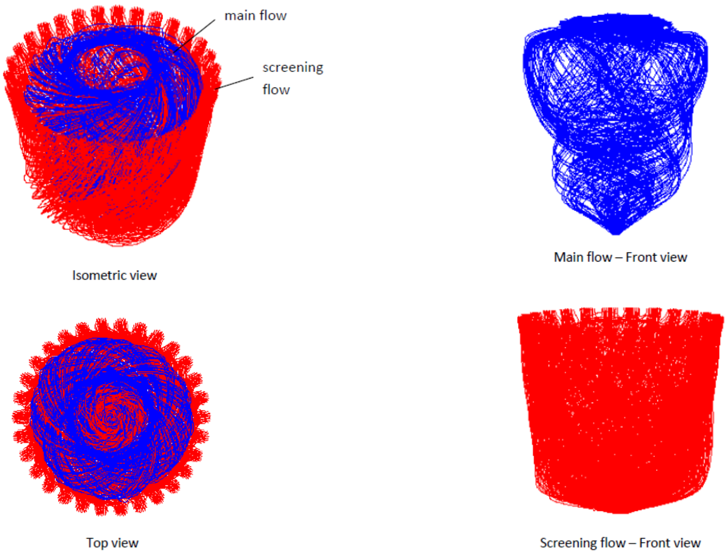


Figure 5 Path lines colored by surface ID

It is seen that the vortex is concentrated in the middle and the pathlines are showing the tracks of carbon particles. This simulation showed us that the flow is rotating as a cyclone, more concentrated swirls, and it is stronger than the vortex in Figure 2. This flow field provides longer residence time, enhanced heat transport, and therefore higher conversion efficiency. However, there is a problem: the wall screening shield is disturbed by the strong vortex, so it does not form a laminar flow as seen in Figure 5. This shows us that guide vanes did help to create better vortex, however, it does not help in keeping the walls clean from carbon deposition because the wall screening flow is literally destroyed by the strong vortex. Now our ongoing research focuses on finding a reactor configuration that can give us a vortex shown in Figure 5 and a laminar wall screening as shown in Figure 2.

Summary of the results and conclusions

Our CFD analysis showed aero-shielded solar cyclone reactor concept creates a flow field where carbon particles make several turns inside the reactor instead of moving towards the exit altogether at a time. In the meantime, wall screening laminar flow keeps the carbon particles away from the wall when they escape from the vortex so they go back to the vortex and then exit the reactor. This shows that carbon deposition on solar reactor wall and carbon clogging at the exit can be solved by this reactor concept. These results also showed us that change in solar reactor design has a significant effect on the flow field which eventually yields change in temperature distribution, and residence time.

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