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► **To cite this version:**

Deewakar Sharma, Arnaud Erriguible, Yves Garrabos, Carole Lecoutre-Chabot, Olivier Nguyen, et al.. Hydrothermal flames at microscale, first observations for DECLIC SCWO study. Colloque Annuel du GDR MFA 2799 (Micropesanteur Fondamentale et appliquée), Comité du GDR MFA 2799, Nov 2022, Hyères, France. 2 p. hal-04154017

HAL Id: hal-04154017

<https://hal.science/hal-04154017>

Submitted on 6 Jul 2023

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Hydrothermal flames at microscale, first observations for DECLIC SCWO study

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With ever growing space activities and deep space missions involving humans expected in coming years, there is a need to develop technologies for sustaining life aboard these space human missions. One such essential technology is means to treat human/organic waste for which using supercritical water oxidation (SCWO) using hydrothermal flames was proposed in this project. The initial objective has been to demonstrate the feasibility of such process at microscale, the requirement favored by size and weight and space constraints in space missions.

The work is done at ICMCB with the support of the CNES postdoc Deewakar Sharma. An experimental setup, for the study of hydrothermal flames during SCWO process, was built around the use of microreactors. The design of these latter has first been incorporated in in-house CFD code, NOTUS, along with a combustion model. The work then has focused on performing experiments under real conditions and assist their understanding via modeling/simulations.

Initial tests have used semi-transparent silicon-pyrex system to check for mixing between ethanol and oxidizer stream along with ensuring H_2O_2 decomposes well into water and oxygen. Subsequently, experiments were performed using sapphire based reactors, fully transparent. The numerical modeling approach was used to comprehend the observations, primarily to identify the conditions for simple oxidation reaction and hydrothermal flame.

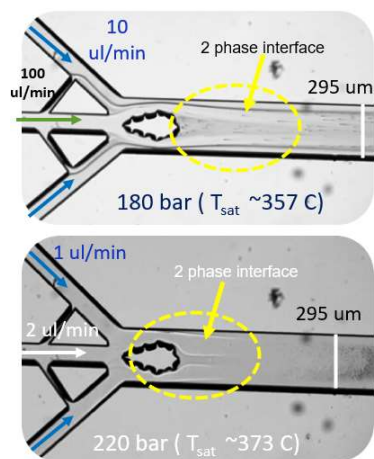
Results

Fig. 1: 2 phase flow in pure water

In order to capture oxidation/flame, one of the key conditions is to ensure that fluid temperature reaches supercritical temperature. While this is not straightforward in the current setup, an intuitive approach was adopted to estimate the safe input temperature conditions to attain that temperature for wide range of flow rates. Knowing the saturated temperature of water at a given pressure, change of phase for a given input temperature ensured that at least saturated temperature has been achieved. This is illustrated for one case in Fig. 1 for $P = 180$ & 220 bar. The observation can be explained as follows: at low flow rates, the fluid gets sufficient time to heat up to the desired saturation temperature and thus, undergoes a phase change (becomes vapor) while at high flow rate, it enters the main channel as a superheated liquid resulting in the observed interface between the two phases.

Subsequently, experiments with real conditions (water + ethanol and water + hydrogen peroxide) were carried out to observe the formation of flame, if any. Through visual observations, thin blue regions (Fig. 2) in the mixing region were observed. It is known that the ethanol burns with blue flame due to excited CO_2 formed as a product. The experiments were thus able to successfully demonstrate capturing the oxidation reaction. However, the question worth pondering is whether it was a simple oxidation reaction or formation of flame. This

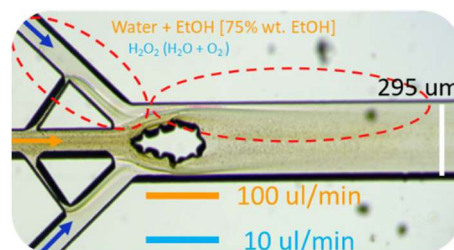


Fig. 2: Thin blue regions corresponding to oxidation of EtOH

can be explained via modeling approach as shown in Fig 3. It can be seen that at inlet temperature 350 C (~ as in experiments), the formation of products (CO₂) leads to very small increase in temperature while injecting at ~400 C results in a significant temperature increase (~200C). Thus, the latter case

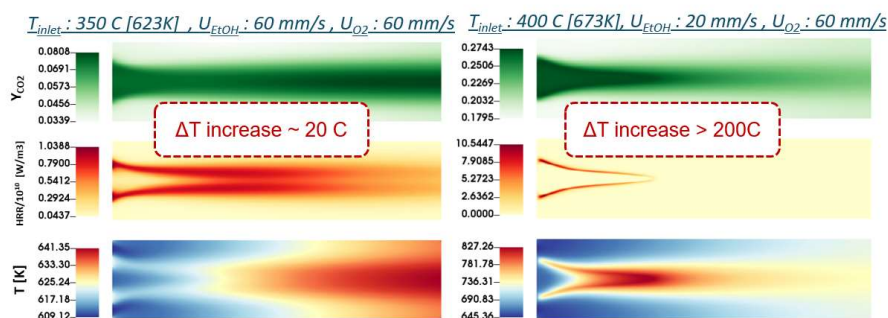


Fig. 3: Different modelling supports showing the influence of the inlet temperature leading to reaction temperature increase

corresponds to flame ignition (further justified by sudden change in heat release rate in the domain as shown in Fig. 3) while the former, as observed in experiments can be categorized as the oxidation reaction. In order to gain a rough

estimate of conditions favoring ignition, a machine learning based approach was sought and various classification models were fitted to predict the same.

Perspectives

The future perspective and challenges to attain the formation of flame at microscale are presented herein. While the current work suggests that realization of such a process is quite within the reach in the current framework, however a more scientific approach, rather than heuristic can aid in attaining the goals more efficiently. The key challenge herein lies to ensure that temperature of the fluid reaches the supercritical conditions once it enters the main reaction channel. One of the simplest means could be to increase the temperature at the heating element which would require to ensure that the microreactor can sustain even harsher temperature conditions. Alternatively, minimizing the heat loss due to convection is of utmost importance. This can be addressed by creating a small chamber to encompass the microreactor or a small window to cover microreactor part exposed to camera. However, while doing so it must be kept in mind not to create temperature gradient across bottom and top surface which could mechanically be unfavorable for the chip. Another approach that could be helpful, at least for experiments on ground, is to preheat the fluids streams before they enter the reactor. This can be achieved by implementing a hot compression part heated at 400-450° C, which was recently developed by ensuring sealing with gold O-rings instead of polymeric ones. This would permit to easily control the heat loss in the reaction zone and provide more flexibility in controlling the inlet temperature. Lastly, the current work was carried out in 2D based reactor system. As a future perspective, it could be interesting to extend this to a 3D microreactor wherein the key challenge lies in etching the same sapphire chip with different depths and aligning them thereafter.

Publications

D. Sharma, A. Erriguible, O. Nguyen, C. Lecoutre, Y. Garrabos¹, U. Hegde, M. Hicks, S. Marre. A preliminary investigation of microreactor designs for supercritical water oxidation using hydrothermal flames for space applications. ISSF, Montreal, May 15-18, 2022.

In preparation:

D. Sharma, A. Erriguible, O. Nguyen, C. Lecoutre, Y. Garrabos, S. Marre, Hydrothermal flames at microscale

D. Sharma, A. Erriguible, O. Nguyen, C. Lecoutre, Y. Garrabos, S. Marre, Effect of gravity on SCWO/hydrothermal flames

D. Sharma, A. Erriguible, O. Nguyen, C. Lecoutre, Y. Garrabos, S. Marre, Predicting ignition conditions for hydrothermal flames using machine learning