



The 7th International Conference on Applied Energy – ICAE2015

Numerical model to design a thermochemical storage system for solar power plant

S. Tescari^{a*}, G. Lantin^a, M. Lange^a, S. Breuer^a, C. Agrafiotis^a, M. Roeb^a, C. Sattler^a

^aGerman Aerospace Center (DLR) – Institute of Solar Research, Linder Höhe, Cologne 51147, Germany

Abstract

Storage of the heat is one of the key points in the development of concentrated solar power plants. Although at an early research stage, thermochemical storage offers several advantages, as for example high energy density, long term storage or high storage temperature. A new concept, in which the reactive material is shaped in a structured, monolithic shape, through which air can flow, was lately proposed. This new concept, exhibiting high surface area and good heat transfer properties, was successfully tested in lab-scale. The next step is the installation of a prototype reactor in an existing solar facility. The definition of the design of such a reactor, as well as the nominal operating conditions, is made through a CFD numerical model, developed and described in this study. A typical charge and discharge cycle is analyzed and used to define the operating conditions. Through simulations, the optimal design and shape of the reactor (height to length ratio, distributor shape, etc.) is defined. The optimization method, defined for this process, shows the importance of the flow uniformity on the reactor performances. The pressure drop threshold, needed to obtain a uniform flow, is found and the reactor shape is defined accordingly.

© 2015 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

Peer-review under responsibility of Applied Energy Innovation Institute

Keywords: Thermochemical heat storage, honeycomb, solar power plant, reactor design

1. The thermochemical storage system

Thermochemical energy storage represents a real challenge on the development of a solar-energy-based economy. The basic idea of the process is to use the concentrated solar thermal energy during high irradiation hours, to drive an endothermic chemical reaction (“charging” phase). If this reaction is completely reversible the thermal energy can be recovered completely by the reverse reaction taking place during off-sun operation (“discharging” phase).

* Corresponding author. Tel.: +49-(0)2203-601-2402; fax: +49-(0)2203-601-4141.
E-mail address: Stefania.Tescari@dlr.de.

Although it is still at an early research stage, the several advantages offered by this storage mode match the needs of the future generation solar power plants. For example, the efficiency of a solar power plant can be increased by increasing the operating temperature. In existing commercial plants, the storage temperature is limited by the thermal stability of the molten salts (lower than 600°C) employed as the storage medium. Thermochemical heat storage can ideally provide for much higher temperatures depending on the chemical reaction chosen [1]. Equally important is the very high allowable energy density, the theoretically constant temperature, at which the storage could be discharged and the possibility of long term storage.

Several reversible reactions with significant heat effects have been proposed for exploitation and studied until now [1]; Among such reactions, reduction-oxidation (redox) reactions involving metal oxides like manganese [1,2], copper, cobalt [3-5] etc. are most attractive for large-scale deployment especially in Solar Power plants that use air as the heat transfer fluid, since these reactions use oxygen as reactive gas, which can be supplied by ambient air, avoiding thus the necessity of storing the gas. Recent studies indicate that cobalt oxide ($\text{Co}_3\text{O}_4 \rightarrow 3\text{CoO (s)} + 0.5\text{O}_2 \text{ (g)}$) seems one of the most promising materials for this application due to several reasons: its redox temperature range is perfectly suitable for new solar tower power plants (equilibrium temperature in air is about 900 °C under atmospheric pressure), the energy density for complete conversion is high (844 kJ/kg) and its performance does not decrease during cycling [4].

The feasibility of this process was already shown in literature, using a solar-heated moving particle reactor [3]. This concept presents several advantages (high surface area, possibility of transporting the material) but also several disadvantages as moving parts at high temperature.

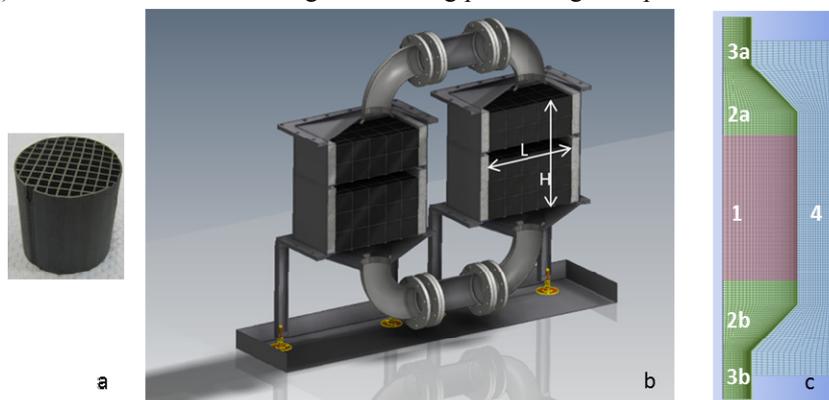


Fig. 1: a) Reactive material structured as honeycomb. b) Sectional view of reactor chambers The black centre is the reactive core (height H and length L) made of honeycomb bricks shown in a). c) Computational domain of one reactor chamber

Literature shows some studies on high temperature thermochemical storage, but mainly limited to packed bed reactor. Challenges of this system are to obtain good air distribution along the bed and sintering of the reactive material. These points could be improved by a novel alternative concept: the reactive material is shaped in a structured, monolithic shape, through which air can flow [6, 7]. This concept exhibits high surface area and good heat transfer properties, preserving the simplicity of the system. In the present study the chosen shape is honeycomb-bricks, as the one shown in Fig. 1a. The honeycomb, dimensioned in a previous study [8] (wall thickness 2,3mm and cell density of 47cells per square inch-cpsi), will have cubical shape of 100mm side, stacked together to form the reactor core.

The final reactor (Fig. 1b), is composed by two identical chambers, each containing a reactive core of about 250kg cobalt oxide in honeycomb shape. During operation the hot air, ideally coming from the solar

receiver, flows through the storage assembly, transferring heat to the solid material, which first heats up (sensible storage) and then undertakes an endothermic chemical reaction (chemical storage). During “discharging” (off-sun) operation, the air flow is reversed: “cold” air is introduced in the storage medium to be heated by the exothermic oxidation reaction, before sent to the power block.

2. The numerical model

A numerical model, developed using the commercial software ANSYS FLUENT, simulates the previously described reactor during charge and discharge. Due to the novelty of the reactor, this model is the first describing its behavior. The objective is to study the impact of the geometry and of the operating condition, by investigating mass and heat transfer as well as the propagation of the reaction in the system.

In order to reduce the computational effort, only one of the 2 chambers is modeled by an axisymmetric 2D model. The symmetry axis is the horizontal boundary on the left side in Fig. 1c. The computational domain is divided in about 17000 quadrilateral cells with increased refinement close to the interfaces. This mesh resolution allows obtaining grid-independent results, in a reduced computational time.

The domain can be divided in 3 zones: a fluid zone (2+3), a porous zone (1) and a solid zone (4). The air enters through the pipe (3a) on the top, passes through a distributor (2a) before flowing through the reactive honeycombs (1), where the reaction takes place. The gas then passes through a second funnel (2b) before exiting the reactor through the pipe (3b) on the bottom in Fig. 1c. All these zones are surrounded by insulating material (4), where no mass, but only heat is exchanged. The reaction zone (1) is the core of the system. Here the honeycomb-shaped reactive material, exchanges heat and oxygen with the gas (air), allowing the chemical reaction. The reactive zone is modeled as an equivalent porous medium characterized by void fraction, specific surface area, anisotropic permeability and anisotropic thermal conductivity (corrected to consider the effect of radiation). A complete simulation of every channel, with the adjacent thin walls, would require a very fine mesh resolution and a computational effort too high for the scope of this study. As solid and fluid phases are not in thermal equilibrium (heat is transferred between them), a dual cell approach is used: a solid zone spatially coincident with the porous fluid zone is defined. This solid zone only interacts with the fluid through heat transfer. The conservation equations for energy are solved separately for the fluid and solid zones with an additional convection heat transfer term between the fluid and the solid. During the reduction reaction, solid cobalt oxide Co_3O_4 is consumed to form solid CoO and oxygen. The modelling of a redox reaction of solid species is not a straightforward task as a reaction consuming a solid material is not supported by FLUENT. Hence the redox reaction is modelled as a surface reaction, assuming that all cobalt oxide species are deposited on the surface of the porous medium. The reaction rate is implemented with the help of a user-defined function.

The gas inlet (upper horizontal boundary in Fig. 1c) has an imposed velocity, composition and temperature. The temperature is kept constant during one phase (higher for the charging phase and lower during discharge). The gas outlet (the horizontal boundary on the bottom) has a pressure outlet condition. The external boundaries of the insulation zone exchange heat with the environment through convection and radiation. In zone 1, the insulation is thermally coupled with the solid cells, while the interface between fluid cells and insulation is adiabatic. The porous zone is connected to the fluid through porous jump conditions.

3. Typical charge and discharge

A typical result of a complete charge and discharge cycle is shown in Fig. 2a, where the nominal operation is simulated. In nominal operation, 250kg of Cobalt oxide, initialized at a temperature of 900K, are charged and discharged by a 0.07kg/s flow of air. During charge, the gas enters (black dotted line, left

axis) at constant high temperature of 1273K and releases its energy to the storage medium. During discharge, the “cold” air at 1000K enters the system and absorbs the energy released by the storage medium. The black curve delineates the temperature evolution of the outlet gas (left axis) and the red dashed one shows the advancement of the reaction (right axis). The cycle can be divided in 7 sub-phases, named from A to G. The sub-phases A-D represent the charging. In E no air flows through the reactor. Phases F-G represent the discharge phase. First the storage is heated, up to the reaction temperature (sub-zone A+B). B represents the transition zone where air with $T > T_{\text{initialization}}$ reaches the outlet. Afterwards the outlet gas temperature has an almost constant zone, where the energy transported by the air is mainly used for the chemical reaction (C). A second transition zone appears (D) when the temperature front with $T > T_{\text{eq}}$ reaches the end of the reactor outlet. After completion of reaction (end of D), hot air flows for 1h more (E), before beginning the discharging phase. At first, the chemical heat is transferred to the air at a relatively constant temperature (F), close to T_{eq} . When the temperature front with $T < T_{\text{eq}}$ reaches the reactor outlet, the temperature declines rapidly before the discharge ends (G). With these inlet temperature values, the reactor is charged in approx. $t=3$ h and discharged in 1.25h.

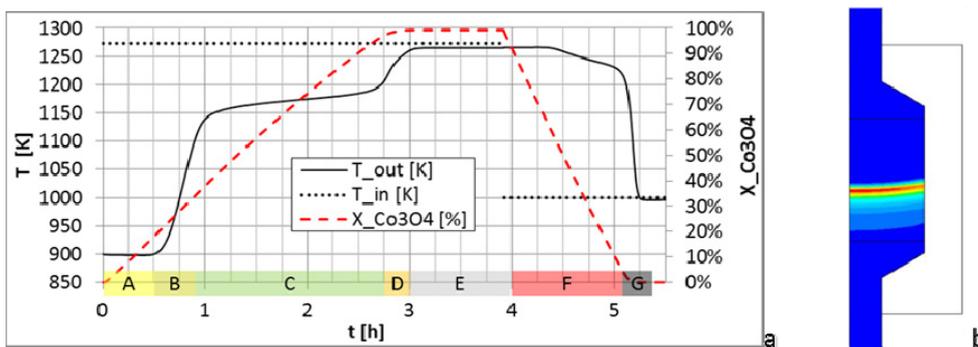


Fig. 2: a) Simulation results for complete charge and discharge cycle at nominal operation. b) Reaction rate during the reduction phase under maximum load conditions. The blue indicates a reaction rate of 0 kmol/m³s and red the highest reaction rate

In a perfect operation the transition zones B, D and G would be very small as this would imply that the storage can be charged and discharged at a relatively constant temperature and that the loss of high exergetic heat is avoided. This can be better understood from Fig. 2b, which shows the reaction rate (blue indicates a reaction rate of 0 kmol/m³s and red the highest reaction rate) at a given time step during the reduction phase. In an ideal case, the reaction should advance in a straight horizontal line moving toward the outlet. If the reaction front has a parabolic shape, as in figure, the lowest sides of the reactor will react with a delay in respect to the center. During this delay, the energy transported by the hot air flowing in the reactor center will be lost. The more parabolic the reactor front is, the more inclined will be the transition zones and the more energy will be lost during charging and discharging. The uniformity of the reaction front is mainly determined by the distribution of the axial flow in the cross section of the reactor.

4. Optimal geometry

As shown above, the flow uniformity inside the reactive zone has a primary role on the good operation of the system. Hence an analysis of the flow distribution inside the reactor, will define its optimal design.

As a measure for the flow uniformity on different cross-sectional planes of the storage, the uniformity index γ is used [9]:

$$\gamma = 1 - \sum_{i=1}^n \omega_i / 2n; \quad \omega_i = |v_i - \bar{v}| / \bar{v} \quad (2)$$

where n is the number of nodes on the evaluation plane, v_i the local axial velocity and \bar{v} the average velocity on the same plane. The uniformity index ranges from 0 to 1 (1 means completely uniform flow).

The first and most important geometrical parameter analyzed is the reactive material shape, i.e. the axial to radial dimension ratio H/L (shown in Fig. 1b).

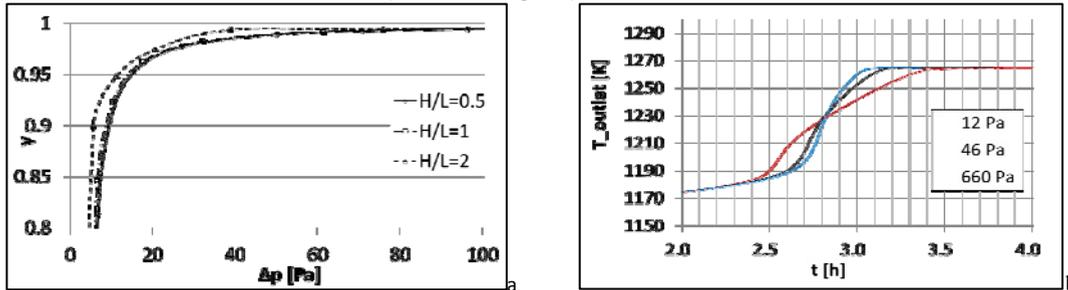


Fig. 3: a) Effect of the inventory pressure loss and the H/L ratio on the flow uniformity. b) Performance of the base case reactor with different pressure losses in the inventory section (Zone D)

Fig. 3a shows the uniformity factor in the central plane of the reactive zone for different pressure losses (corresponding to different permeabilities of the porous medium) and for 3 different H/L ratios. The flow is analyzed through steady state simulation including heat losses but neglecting the chemical reaction. The curve shows a strong decrease of flow uniformity below a pressure loss of about 40 Pa, for every H/L ratio. A more slender design (high H/L ratio) yields higher uniformity. For H/L=2, a pressure loss of 50Pa assures a high flow uniformity. For this case, Fig. 3b shows a part of the charge cycle (Zone D in Fig. 2a) for different pressure losses, through transient simulations. As already mentioned, the ideal operation of the system has almost vertical transition zones. The negative effect of a low pressure loss (12Pa) on the performance is clearly recognizable, while the difference between 46 and a very high Δp (660Pa) has a much smaller importance. For pressure drop higher than 80 Pa, high and constant value of the uniformity factor is insured, independently on the shape.

High pressure loss leads on one hand to good flow distribution, on the other hand to high parasitic losses, necessary to pump the air through the system. Thus the minimal pressure drop allowing a uniform flow has to be chosen. Considering the gas flow variation range (0.0065 – 0.13 kg/s) of the experiment and in order to operate efficiently in 10 to 90 % of this operation range, a minimum H/L ratio for the reactor of H/L=0.76 can be calculated. Below the minimal H/L ratio the pressure loss drops below 80 Pa, leading to flow maldistribution (result valid for the operating condition and the material described above). In the same way, other parameters are investigated as the distributor height and angle, empty space before and after the reactive material, pipe dimension and others. It was shown that, when a pressure drop of 80Pa is assured (for example with a H/L ratio higher than 0.76), they have only marginal importance in the flow distribution. Therefore these parameters are chosen depending on different considerations.

5. Reactor design

The reactor consists of two equal chambers (Fig. 1 b), each having a total height of around 1.6 m and about 0.6 m side, in square surface. The reactive core, made of cobalt oxide honeycombs of 8.5 cm side, is shaped accordingly to the results presented above, with a H/L higher than 0.76. As the funnel-shaped gas distributor and collector don't lead to any performance improvement (as shown in the previous section), they are replaced by a squared shape above and behind the reactive part. This shape is much

easier to produce. Although the empty volume was also not beneficial for the reactor operation, a 5cm-height empty volume was added to improve the flow distribution above the reactive zone and to allow the expansion of the material. This space is also included at the bottom to eventually remove falling particles. A parallel mechanical study [8] showed the importance of minimizing the mechanical stress experienced by the reactive material on the support surface. Therefore, a second holding net, made of high alloy steel, is implemented in the middle of the honeycombs. The diameter of the inlet pipe, having only marginal influence on the flow distribution, is chosen according to DIN norms to 163.1mm, in order to don't exceed 25m/s air speed.

High performance insulation (microporous material), not included in the figure, will surround the reactor.

6. Conclusion

A novel and promising thermochemical storage system consists on shaping the storage material in structure form as honeycomb. In order to design and dimension a thermochemical storage prototype, this study develops a CFD model able to study the system performance, to optimize the design of the storage reactor and to define the operating conditions.

First a typical charge and discharge phase are analyzed, allowing the definition of the operating condition of the system. Secondly, the models allows to define the optimal system geometry (height/length ratio of the reactive core, distribution system, etc.). The flow uniformity results to be a key factor for the reactor performance. The pressure drop, needed to obtain a uniform flow, is found and the reactor shape is defined accordingly. The results are used for building a thermochemical storage system prototype, which will be implemented for the first time in an existing solar facility (Solar Tower Jülich).

Acknowledgements

The authors would like to thank the European Commission for partial funding of this work within the Project RESTRUCTURE –contract n° 283015” under the Energy 2011.2.5.1 Call. and within the Project “FP7-PEOPLE-2011-IEF, 300194” under the Fellowship Marie Curie Actions.

References

- [1] Wong, B., Thermochemical heat storage for concentrated solar power: General Atomics Report GA–C271372011.
- [2] Stobbe, E.R., de Boer B.A., and Geus J.W., The reduction and oxidation behaviour of manganese oxides. *Catalysis Today*, 1999. 47(1-4): p. 161-167.
- [3] Neises, M., Tescari S., de Oliveira L., Roeb M., Sattler C., and Wong B., Solar-heated rotary kiln for thermochemical energy storage. *Solar Energy*, 2012. 86(10): p. 3040–3048.
- [4] Agrafiotis, C., Roeb, M., Schmücker, M., Sattler, C., 2014b. Exploitation of thermochemical cycles based on solid oxide redox systems for thermochemical storage of solar heat. Part 1: Testing of cobalt oxide-based powders. *Solar Energy* 102, 189-211.
- [5] Tescari, S., Agrafiotis, C., Breuer, S., de Oliveira, L., Puttkamer, M., Roeb, M., Sattler, C., 2014. Thermochemical Solar Energy Storage Via Redox Oxides: Materials and Reactor/Heat Exchanger Concepts. *Energy Procedia* 49, 1034-1043.
- [6] Pagkoura, C., Karagiannakis, G., Zygogianni A., Lorentzou S., Kostoglou M., Konstandopoulos G.A., Rattenbury M., Woodhead W.J. Cobalt oxide based structured bodies as redox thermochemical heat storage medium for future CSP plants. *Solar Energy*, 2014. 108(0): p. 146-163.
- [7] Karagiannakis, G., Pagkoura, C., Zygogianni, A., Lorentzou, S., Konstandopoulos, A., 2014. Monolithic Ceramic Redox Materials for Thermochemical Heat Storage Applications in CSP Plants. *Energy Procedia* 49, 820-829.
- [8] Tescari, S., Breuer S., Roeb M., Sattler C., Flucht F., Schmücker M., Karagiannakis G., Pagkoura C., and Konstandopoulos A. G., Design of a thermochemical storage system for air-operated solar tower power plants. in *SolarPACES 2014*. 2014. Beijing, China: Energy Procedia.
- [9] Zunft, S., Dreißigacker, V., Hahn, J., Kammel, J. Flow Distribution Calculations in Regenerator-Type Heat Storage for Solar Tower Plants. in *SolarPACES*. 2011. Granada.



Biography

Stefania Tescari was born in Italy in 1981, graduated in Physics at the University of Padova, and has a PhD on optimization of reactor design from the University of Perpignan, France. At present she works as a researcher in the solar research institute at the German Aerospace center (DLR), Cologne.