Monte Carlo method to calculate the lifetime efficiency of a solar reactor for reduction of zinc oxyde

O Farges, Jean-Jacques Bézian, M El Hafi

▶ **To cite this version:**

O Farges, Jean-Jacques Bézian, M El Hafi. Monte Carlo method to calculate the lifetime efficiency of a solar reactor for reduction of zinc oxyde. 2016 AIChE Annual Meeting, Nov 2016, San Francisco, France. hal-04113074

HAL Id: hal-04113074
https://hal.science/hal-04113074

Submitted on 2 Jun 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Monte Carlo method to calculate the lifetime efficiency of a solar reactor for reduction of zinc oxyde

O. Farges, J.J.Bézian, and M. El Hafi

Université Fédérale de Toulouse Midi-Pyrénées, Mines Albi, UMR CNRS 5302, Centre Rapsodee, Campus Jarlard, f-81013 Albi ct cedex 09, France

Commonly used to produce electricity through thermodynamic cycles (Gemasolar Power Plant, Ivanpah Solar Power Plant, ...), concentrated solar plant can also be seen as an alternative to fossil fuel-based methods for H_2 generation [5]. High temperature solar thermochemical processes make use of concentrated solar energy to achieve metal oxydes reduction. These processes can be seen as a solar energy storage : products may be stored and transported (H_2 in this case). Among all metal oxydes reduction, the zinc oxyde to zinc (ZnO/Zn) REDOX reactions are particularly attractive as the first part of a two step water splitting cycle (eqs. (1a) and (1b)).

As presented on fig. 1, a thermochemical reactor $\mathcal{R}$, placed at the top of a solar tower receives concentrated solar energy emmited from the sun $\mathcal{S}$ and reflected by heliostats $\mathcal{H}$. Thus, the reactor, feeded with zinc oxyde, reaches high temperature, *ie* above 1400 K, to achieve reduction of zinc oxyde and to procude zinc Zn.

$$\mathrm{ZnO} \rightarrow \mathrm{Zn} + \frac{1}{2}\mathrm{O_2} \tag{1a}$$

$$\mathrm{Zn} + \mathrm{H_2O} \rightarrow \mathrm{ZnO} + \mathrm{H_2} \tag{1b}$$

In order to evaluate the performance of a thermochemical solar plant and to allow an optimally design of both the reactor and the whole facility (heliostat field,

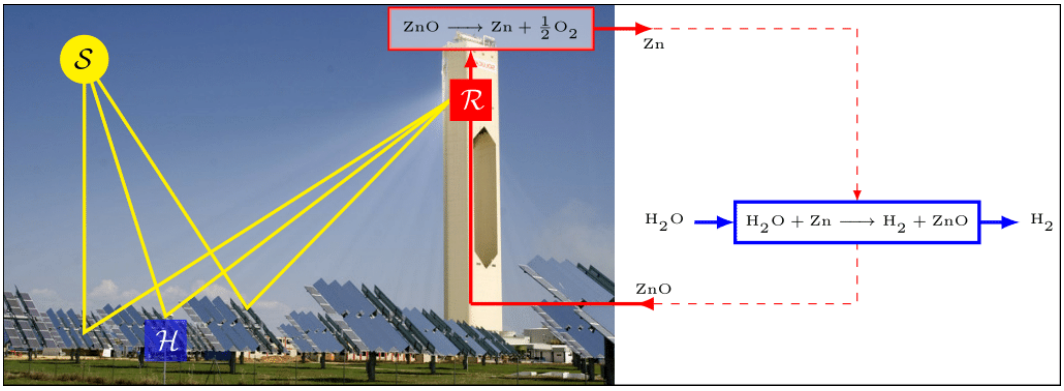

Figure 1: H_2 solar production process

tower), numerical modelling of this process is needed. We present here a Monte Carlo algorithm that allows to estimate the solar plant annual productivity. This algorithm associate the thermodynamical knowledge of the non-linear kinetics of zinc oxyde dissociation to the description of the radiative transfer on a multiple-reflection central receiver solar plant. This algorithm deals with non-linearity due to coupling between photon transport and the metal oxyde reduction reaction although it was identified that "the extension of Monte Carlo methods to nonlinear processes may be impossible" [1]. Moreover, the widespread opinion is currently that "Monte Carlo methods are not generally effective for nonlinear problems mainly because expectations are linear in character"[3].

To evaluate the quantity of interest, *ie* the annual solar-to-chemical conversion rate $\langle \eta_r \rangle$, this Monte Carlo algorithm firstly computes the instantaneous power received at the entrance of the reactor at an instant $\boldsymbol{i}$, $\langle P_{th}(\boldsymbol{X}|\boldsymbol{i}) \rangle$. A Monte Carlo algorithm previously presented in [2] is used as a first step of the proposed algorithm to evaluate this quantity. The random variable $P_{th}(\boldsymbol{X}|\boldsymbol{i})$ is the contribution of optical paths $\boldsymbol{X}|\boldsymbol{i}$ to the thermal power collected at instant $\boldsymbol{i}$. Then, $\langle P_{th}(\boldsymbol{X}|\boldsymbol{i}) \rangle$, the expextation of this random variable, is the instantaneous thermal power collected at moment $\boldsymbol{i}$. A part of the power received by the reactor, the instantaneous useful power $P_u = f\left(P_{th}(\boldsymbol{X}|\boldsymbol{i})\right)$, represents the efficient energy used to achieve REDOX reactions with an instanteneaous reaction rate described by a zero-order Arrhenius-type law, strongly non-linear. Integration over time of the instantaneous conversion rate leads to the lifetime conversion rate $\langle \eta_r \left(\langle P_{th}(\boldsymbol{X}|\boldsymbol{i}) \rangle \right) \rangle_{\boldsymbol{i}}$ as presented eq. (2).

$$\langle \eta_r \rangle = \int_{LifeTime} \frac{P_u(t)}{P_{th}(t)} \tag{2}$$

The Monte Carlo algorithm is based on a Taylor expansion of $\langle \eta_r \rangle$ around $P_{th0} >$

$P_{th}(\boldsymbol{X})$. Independent and equally distributed optical-path random variables $\boldsymbol{X}_j|\boldsymbol{I}$ are introduced and the infinite power series is statistically formulated thanks to the discrete random variable J whose realization j is the order of Taylor expansion. The Taylor expansion is stopped through a Bernoulli process in order to decide whether the algorithm stops or continues without introducing a statistical bias.

Some simulations are made with the 1 MW reactor presented in [4]. A simplified model of thermal losses is applied and a comparison of the nominal performance between results obtained with the Monte Carlo algorithm and experimental results presented in [4] are presented in table 1. The difference between the measured and calculated results are due to the simplified thermal losses model as well as uncertainties of the measurements.

Table 1: Size and performance of a 1 MW reactor

Parameters	**Units**	**Values**
Aperture diameter	mm	600
Window diameter	mm	790
Cavity diameter	mm	1600
Cavity length	mm	2400
Conversion rate η_r [4]	%	54
Conversion rate estimated η_r	%	40.2
Annual conversion rate $\langle\eta_r\rangle$	%	4.8

In the final paper, more results will be presented as well as the complete mathematical formulation of the proposed algorithm and a more accurate thermal losses model.

References

[1] J. H. Curtiss. monte carlo methods for the iteration of linear operators. *Journal of Mathematics and Physics*, 32(1):209–232, 1953.

[2] O. Farges, J. Bézian, H. Bru, M. E. Hafi, R. Fournier, and C. Spiesser. Lifetime integration using monte carlo methods when optimizing the design of concentrated solar power plants. *Solar Energy*, 113(0):57 – 62, 2015.

[3] M. H. Kalos and P. A. Whitlock. *Monte carlo methods*. John Wiley & Sons, 2008.

[4] L. Schunk, W. Lipiński, and A. Steinfeld. Heat transfer model of a solar receiver-reactor for the thermal dissociation of zno-experimental validation at

10 kw and scale-up to 1 mw. *Chemical Engineering Journal*, 150(23):502 – 508, 2009.

[5] A. Steinfeld. Solar thermochemical production of hydrogen—-a review. *Solar Energy*, 78(5):603–615, 2005.