

## A Smart Solar Reactor for Environmentally Clean Chemical Processing

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Solar thermal process reactors can convert intermittent solar radiation and reactants into energy dense, storable and transportable chemical fuels. This method uses concentrated solar energy as the source of high temperature process heat for the production of many commodities such as zinc, cadmium, magnesium, hydrogen and carbon with zero or minimal emissions. Transient inefficiencies due to natural fluctuations in solar radiation degrade product throughput in all solar reactors. It is therefore important to design a system that allows the reactor to respond to environmental factors in order to maintain semi-constant temperatures inside the reactor. Maintaining reactor operating conditions stabilizes process efficiency. Previously, the effects of various aperture geometries have been investigated through the use of ray-tracing and discrete ordinance numerical simulations. In this paper, a more complete concept for the aperture mechanism entitled the “sliding variable aperture” is presented. This variable aperture allows the solar reactor to dynamically respond to changing flux conditions. Optical simulations have been carried out in conjunction with a numerical method for determining the output of the reactor with a dynamic aperture and changing flux conditions. Historical weather data was gathered from the National Renewable Energy Laboratory (NREL). Convective losses were modeled based on a desired isothermal temperature and static standard operating environmental temperatures. Results from the optics simulations, reaction kinetics and the heat transfer model were used to find the range for the area of the gap for the aperture mechanism, which resulted with ranges between 13.8 to 52.3 cm<sup>2</sup> for beam normal insolation amounts between approximately 165-1100 W/m<sup>2</sup> in order to maintain a minimum 1500 K internal cavity temperature inside the solar reactor.

### 1. Introduction

Utilization of concentrated solar energy for high temperature chemical processing offers the possibility of reduced or completely emission-free production of hydrogen, carbon black, and metals (Ozalp et al., 2010a). In order to house the solar thermochemical processes a “solar reactor” is needed. However, there are major problems that can affect the performance. The most uncontrollable factor is the natural variations in solar radiation due to weather and environmental conditions as well as the position of the sun. This problem applies to all types of solar reactors because temperature is the most important factor in reactant to product conversion efficiency. If the reactor temperature can be kept constant, then the process efficiency can be kept almost constant regardless of weather conditions. Prior studies on the operating conditions of solar reactors have assumed homogenous and instantaneous temperatures within the reactor (Steinfeld

and Schubnell, 1993). Other studies have simulated realistic environmental conditions based on historical data and investigated the effects of intermittent insolation on the production of a desired output (Charvin et al., 2008). Alternatively, solar simulators have been used (Kogan and Kogan, 2003) as well as outdoor testing in solar furnaces (Abanades and Flamant, 2007; Bertocchi et al., 2004). However, these works do not include the transient nature of solar insolation in their methodologies. Variations in the incident flux upon the reactor are a product of the environment, geometrical design of the concentration system, tracking algorithms and overall concentration ratios. Furthermore, wear and fouling of concentration surfaces and aperture window also affect maximum achievable flux densities. These factors combined are present within any solar concentrator and each serve to decrease efficiency. It is therefore important to design a system that allows the reactor to respond to environmental factors in order to maintain semi-constant temperatures inside the reactor.

The idea of maintaining isothermal internal conditions is not novel; several geometrical, surface coating and unique concentration methods have been proposed. These include specular internal coatings (Fletcher and Steinfeld, 1987), and different reactor geometries (Tan et al., 2008). Theoretical and experimental studies on the flux image produced by concentrating systems have been highly investigated (Daly, 1979; Hong and Lee, 1987; Ulmer et al., 2002). One of the most significant efforts to design a cavity that attempts to maintain quasi-equilibrium is outlined in a US design patent issued in 1980 for an aperture control device for use with solar thermal concentrators (Jubb, 1980). The proposed device was made up of at least three aperture blades, each with an embedded thermocouple. The blades were actuated individually by separate servo motors. The stimulus for changing the aperture was decided as the temperature at the leading edge of each aperture blade. While the patent correctly describes the need to balance reradiated losses with the captured incoming flux, this method of control does not readily allow the maintenance of quasi-equilibrium conditions inside the reactor as the stimulus takes place outside of the reactor cavity. Furthermore, the individual control of each aperture blade complicates requisite control systems with regards to maintaining internal conditions. Another example study on variable aperture mechanisms was done by Galal et al. (1988), where the use of variable apertures in order to modulate the solar energy impinging on a receiver. This variable aperture was used to avoid excessive solar energy waste and avoid the excess radiation and convection losses from the receiver. Previously, the effects of various aperture geometries have been investigated through the use of ray-tracing and discrete ordinance numerical simulations (Ozalp et al., 2010b; Ozalp and Kanjirakat, 2010; Ozalp and Jayakrishna, 2010). Varying the aperture radii allows the reactor to extend the useful beam normal insolation range in which it can acceptably perform by expanding or contracting depending on the insolation flux density and required cavity temperature. With this configuration, the solar cracking reactor can better maintain semi-isothermal internal conditions. A solar reactor that can maintain quasi-equilibrium conditions inside the cavity would avoid the dramatic fluctuations on the reactor performance regardless of the weather conditions.

## **2. Aperture mechanism for maintaining semi-constant temperature**

The aperture consists of eight parts; a gear, a top rack and bottom rack, a top guide and a bottom guide, a guide shield, and two blades. Figure 1 shows the assembled depiction of the concept created in SolidWorks<sup>®</sup>.

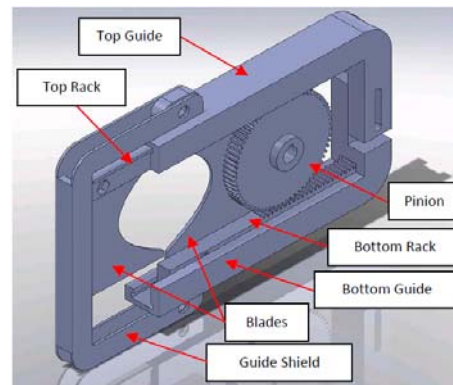


Figure 1: Sliding variable aperture mechanism.

The mechanism continuously varies the aperture area by employing a simple rack and pinion gear system. The pinion gear is mated to the output shaft of a motor; the angular displacement of the motor shaft controls the distance, and therefore area, of the two aperture blades. The requisite area is dependent on the desired internal temperature, incoming flux density, and desired product output. The pinion gear is placed between two racks which run about the top and bottom of the gear. Each of these racks move through a hollow T-shaped guide holding the rack in place. Both guides are held in place by a guide shield and both aperture blades are of the same design. The parabolic curvature of the blades has been designed to allow the aperture to best approximate a circle throughout most of its travel. This sliding mechanism simplifies the dynamics and control of the system, as well as simplifying the manufacturing process. The pinion gear is controlled by a program created in LabVIEW. Although this rack and pinion gearing mechanism has not been used in solar thermal reactors to achieve sliding aperture effect, there exist studies that have utilized similar mechanisms for completely different research purposes. For example, a variable aperture concept is used to allow the passage of a certain aspect ratio of a neutron beam (Hill, 1983). The aperture consists of four blocks hoisted in such a way so that the apexes are in contact. The movement of the blocks is constrained to a square enclosure, where the constrained path will form a square opening in the center proportional to the distance moved by the blocks. Another rack and pinion mechanism was developed by (Sung et al., 2008). The purpose of their mechanism was to effectively control the duty ratio of waveguide grating by controlling the exposure time of an interference beam. In their system a rack is mounted on a shaft which is connected to a motor. The motor causes the shaft to move horizontally thereby enlarging or decrease the aperture.

### 3. Optical methodology

Optical simulations have been carried out in conjunction with a numerical method for determining the output of the reactor in transient flux conditions. First the absorption efficiency is defined as the difference in how much power is intercepted by the aperture and how much power is reradiated through the aperture due to the cavity temperature. This is divided by the total amount of power reflected towards the reactor by the concentration system:

$$\eta_{\text{absorption}} = \frac{\alpha_{\text{eff}} P_{\text{aperture}} - \varepsilon_{\text{eff}} A \sigma T^4}{P_{\text{in}}} \quad (1)$$

where  $\alpha_{\text{eff}}$  and  $\varepsilon_{\text{eff}}$  are the effective absorptance and emittance of the receiver, both equal to 0.95 in this case.  $P_{\text{aperture}}$  is the amount of power intercepted by the aperture,  $P_{\text{in}}$  is the total power reflected by the concentration system,  $A$  is the aperture area,  $\sigma$  is the Stefan-Boltzmann's constant, and  $T$  is the internal temperature of the cavity. Setting  $\eta_{\text{absorption}}$  to zero yields the stagnation temperature, effectively stating that the system is in equilibrium and that the net energy entering the system via the aperture and leaving the system by reradiation is zero. Solving for Eq. (1) yields the reactor steady state temperature,  $T_s$ . Equation (1) therefore above reduces to Stefan-Boltzmann's law, allowing one to calculate the steady state internal temperature, assuming homogenous internal temperature distributions:

$$\alpha_{\text{eff}} P_{\text{aperture}} = \varepsilon_{\text{eff}} A \sigma T^4 \quad (2)$$

However, by definition, the stagnation temperature occurs when no work is being done; the intercepted power is equal to the power being reradiated through the aperture. Thus a modification of (2) is required to allow the application of energy to the chemical reactants.

$$\alpha_{\text{eff}} P_{\text{aperture}} = -\varepsilon_{\text{eff}} A \sigma T_s^4 - \Delta H \dot{m} - h A_{\text{react}} \Delta T - k A_{\text{react}} \Delta T \quad (3)$$

In this model the energy used during the chemical decomposition of methane is now defined as the product of the required change in enthalpy, in this case methane cracking to  $\text{H}_2$ , and mass flow rate. Conductive and convective losses are also considered—if they are not then the apparent stagnation temperature will reach infinity as the aperture area approaches zero. Optical simulations were conducted using TracePro<sup>®</sup>, which was employed to determine the intercepted flux images. TracePro<sup>®</sup> utilizes a stochastic non-sequential script in its Monte Carlo ray tracing algorithm. Chemical solar-to-hydrogen efficiency, which is the ratio of the generated chemical energy of the product fuel to the total fed energy, is calculated from the energy model as follows:

$$\eta_{\text{STH}} = \frac{U_{\text{H}_2} j_{\text{H}_2}}{-\varepsilon_{\text{eff}} A \sigma T_s^4 - \Delta H \dot{m} - h A_{\text{react}} \Delta T - k A_{\text{react}} \Delta T} \quad (4)$$

where  $j_{\text{H}_2}$  is the specific energy density for hydrogen. It is seen that the solar-to-hydrogen efficiency depends mainly on solar flux through the aperture and the reaction kinetics. This is strongly dependent on optimizing (3) for any given incoming flux image.

#### 4. Validation

Optical validations have been carried out using TracePro and the above Equation (3). The data set used was appropriated from openly available measurements from the National Renewable Energy Laboratory (NREL). Two days were chosen: July 5<sup>th</sup> and July 27<sup>th</sup> of 2010. These two days represent a “clear” and a “cloudy” day. The flux distribution was modeled as a collimated source with a concentration system similar to that as experimentally used by Steinfeld and Schubnell (1993). That is, the source was modeled as a collimated Gaussian circular distribution with a standard deviation of 5.2cm and a reflected power of 18.9kW. Convective losses were modeled based on a desired isothermal temperature and room temperature environmental operating conditions under natural convection. Internal wall temperatures were considered as the same temperature of the cavity temperature. Heat was conducted through the cavity, through the insulation, and then dispersed through natural convection. A similarly sized experimental reactor, which was maintained at similar temperatures, was found from a study by Bertocchi, et al. in which the wall materials and thicknesses are discussed.

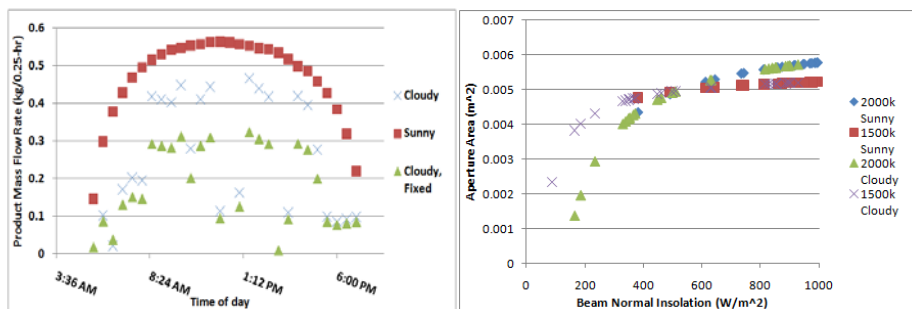


Figure 2: Product mass flow rate output for variable and fixed aperture reactors on cloudy and sunny days

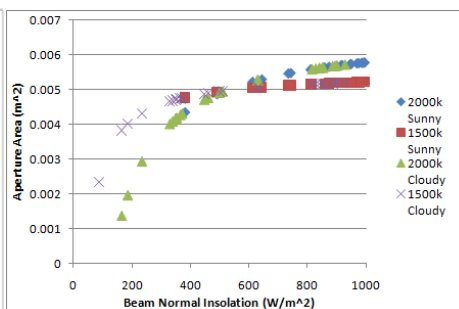


Figure 3: Required aperture area versus insolation amount for sunny and cloudy days in order to maintain different internal temperatures

From Figure 2 it can be seen that the maximum product output occurs when the temperature is at the lower temperature. This is because there is because at this temperature conversion efficiency is still high and there is more energy left over that can be used in the chemical kinetics. The variable aperture design allows the reactor to stay in between at least these two temperature set points on both these days, and shows that it can be adjusted to always allow a maximum of product output. An optimized fixed aperture reactor is also shown, the output of which is slightly higher at low insolation levels but lower at high insolation levels. For the variable aperture over the cloudy day a total of 6.5 kg of hydrogen is produced. During the same time period approximately 4.9 kg is produced by the fixed aperture reactor. During these simulations the aperture area spans a minimum of 13.8 cm<sup>2</sup> to 52.3 cm<sup>2</sup>, or the equivalent of a circular aperture ranging in radii from 2.1 to 4.1 cm. It is also seen in Figure (3) that as the process temperature or insolation amount decreases the aperture radii decreases. The trends in this figure are in agreement with the numerical study performed by Steinfield and Schubnell (1993). This is because the reradiation losses, the largest factor in high temperature reactors, are minimized by the temperature decrease. An optimization needs to be performed for each reactor judging on the temperature, size, reactant, mass flow rate and residence time. The aperture size in this model is strongly dependent on the incoming flux distribution and intensity.

## 5. Summary of the results and conclusions

Optical and numerical simulations have been carried out showing the effect a changing variable aperture can have on internal temperature distributions. The optical simulations and heat transfer model yielded the required aperture range for the reactor to maintain a minimum 1500 K internal cavity temperature. The aperture area varied from 13.8 to 52.3 cm<sup>2</sup> as the flux density changed from 165 to 1100 W/m<sup>2</sup>. In summary, these results show that a change in solar reactor design can have a significant effect on the internal temperature distribution.

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