

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

O. Farges^{1,2}, M. El Hafi¹, J.J. Bézian¹
olivier.farges@univ-lorraine.fr

¹RAPSODEE Center, UMR CNRS 5302, Mines Albi, Toulouse University, France

²LEMETA Lab., UMR CNRS 7563, Lorraine University, Nancy, France

Thursday 17 November 2016

Modelling of a solar reactor plant

Estimation of the lifetime energy conversion efficiency

Monte Carlo modelling

Simulation results

Conclusion and Outlook

Modelling of a solar reactor plant

Estimation of the lifetime energy conversion efficiency

Monte Carlo modelling

Simulation results

Conclusion and Outlook

A MODEL TO SIMULATE THERMOCHEMICAL SOLAR PLANTS

- ▶ To estimate performance over a defined period of time (1 h, 1 day, 1 year or more)
- ▶ To optimally design the reactor and the whole facility (heliostat field, tower, beam down, ...)



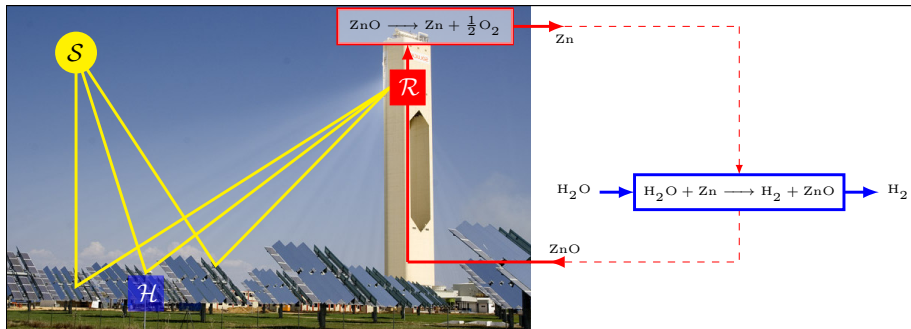
DIFFICULTIES TO BE OVERCOME

- ▶ Take into account the sun's path and the intermittent nature of the solar resource ¹
- ▶ Deal with the nonlinear nature of chemical conversion laws

¹O. Farges et al. "Life-time integration using Monte Carlo Methods when optimizing the design of concentrated solar power plants". In: *Solar Energy* 113 (2015), pp. 57–62

SOLAR ZnO/Zn REDOX PROCESS

A well known thermochemical process²³⁴ as case study



² A. Steinfeld. "Solar thermochemical production of hydrogen—a review". In: *Solar Energy* 78.5 (2005), pp. 603–615

³ P. Haerberling et al. "A receiver-reactor for the solar thermal dissociation of zinc oxide". In: *Journal of Solar Energy Engineering* 130 (2008), pp. 021009–1

⁴ R. Müller, W. Lipiński, and A. Steinfeld. "Transient heat transfer in a directly-irradiated solar chemical reactor for the thermal dissociation of ZnO". In: *Applied Thermal Engineering* 28.5–6 (2008). pp. 524–531

ASSUMPTIONS

Concerning the reactor thermal behaviour

- ▶ The reactor thermal efficiency γ_r is constant

$$\gamma_r = \frac{P_u(t)}{P_{th}(t)} = 80\%$$

- ▶ Conductive and convective losses are not taken into account
- ▶ The reactor is at a uniform temperature T_r

OUTLINES

Modelling of a solar reactor plant

Estimation of the lifetime energy conversion efficiency

Monte Carlo modelling

Simulation results

Conclusion and Outlook

THERMAL POWER EXPRESSION

The thermal power P_{th} could be expressed as a function of the reactor temperature T_r

- ▶ $P_{th}(t) = \frac{A_{aperture} \times \epsilon \times \sigma}{1 - \gamma_r} \times T_r(t)^4$
- ▶ Moving from $P_{th}(t) = f(T_r(t))$ to $T_r(t) = f^{-1}(P_{th}(t))$
- ▶ $T_r(t) = \sqrt[4]{\underbrace{\frac{1 - \gamma_r}{A_{aperture} \times \epsilon \times \sigma}}_{k_T}} \times P_{th}(t)^{1/4}$

INSTANTANEOUS ENERGY CONVERSION EFFICIENCY

- ▶ The instantaneous solar-to-chemical energy conversion efficiency

$$\eta_r(t) = \frac{P_u(t)}{P_{th}(t)} = \frac{\nu(T_r(t)) \times (H_r(T_r(t)) + \Delta H(T_r(t)))}{P_{th}(t)}$$

with

- ▶ the reaction rate $\nu_r(T_r(t))$ is a zero-order Arrhenius-type rate law

$$\nu_r(T_r(t)) = V_r \times k_0 \exp\left(\frac{-E_a}{R \times T_r}\right)$$

- ▶ the reaction enthalpie $H_r(T_r(t))$ and the enthalpie change $\Delta H(T_r(t))$ are polynomial functions of T_r

INSTANTANEOUS ENERGY CONVERSION EFFICIENCY

- ▶ The instantaneous solar-to-chemical energy conversion efficiency

$$\eta_r(t) = \frac{P_u(t)}{P_{th}(t)} = \frac{\nu_r(P_{th}(t)) \times (H_r(P_{th}(t)) + \Delta H(P_{th}(t)))}{P_{th}(t)} = f(P_{th}(t))$$

with

- ▶ the reaction rate $\nu_r(P_{th}(t))$ is a zero-order Arrhenius-type rate law

$$\nu_r(P_{th}(t)) = V_r \times k_0 \exp\left(\frac{-E_a}{R \times k_T} P_{th}(t)^{-1/4}\right)$$

- ▶ the reaction enthalpie $H_r(P_{th}(t))$ and the enthalpie change $\Delta H(P_{th}(t))$ are polynomial functions of P_{th}

LIFETIME ENERGY CONVERSION EFFICIENCY

- ▶ The lifetime solar-to-chemical energy conversion efficiency

$$\langle \eta_r \rangle = \int_{LifeTime} \eta_r(t) dt$$

- ▶ We obtain a formulation where η_r is a combination of several nonlinear functions of the time-dependant thermal power $P_{th}(t)$
- ▶ The aim is now to simulate this model with MC method

OUTLINES

Modelling of a solar reactor plant

Estimation of the lifetime energy conversion efficiency

Monte Carlo modelling

Simulation results

Conclusion and Outlook

WHY WE ARE USING MC METHOD

Main reasons to apply MC method

- ▶ Effective method to deal with multi-integral formulation
- ▶ Orthogonality with geometric aspects
- ▶ Suited for massive parallelization
- ▶ Accurate prediction with confidence interval
- ▶ Sensitivity estimations
- ▶ Easy coupling with a stochastic optimization algorithm⁵

⁵O. Farges et al. "Particle swarm optimization of solar central receiver systems from a Monte Carlo direct model". In: *IPDO 2013 : 4th Inverse problems, design and optimization symposium. IPDO 2013 : 4th Inverse problems, design and optimization symposium*. Ed. by O. Fudvm. I.-L. Battaëlia. G. Dulikravich. et al. Albi. Ecole des Mines d'Albi-Carmaux. June 2013

NON LINEARITIES AND MC METHOD

- ▶ the wide spread opinion:
 - ▶ *“the extension of Monte Carlo methods to nonlinear processes may be impossible”*⁶
 - ▶ *“Monte Carlo methods are not generally effective for nonlinear problems mainly because expectations are linear in character”*⁷

⁶ J. H. Curtiss. *“Monte Carlo” methods for the iteration of linear operators*. In: *Journal of Mathematics and Physics* 32.1 (1953), pp. 209–232

⁷ M. H. Kalos and P. A. Whitlock. *Monte Carlo Methods*. John Wiley & Sons. 2008

NON LINEARITIES AND MC METHOD

- ▶ the wide spread opinion:
 - ▶ *“the extension of Monte Carlo methods to nonlinear processes may be impossible”*⁶
 - ▶ *“Monte Carlo methods are not generally effective for nonlinear problems mainly because expectations are linear in character”*⁷
- ▶ **We propose a method to deal with nonlinear problems with MC method**

⁶ J. H. Curtiss. *“Monte Carlo” methods for the iteration of linear operators*. In: *Journal of Mathematics and Physics* 32.1 (1953), pp. 209–232

⁷ M. H. Kalos and P. A. Whitlock. *Monte Carlo Methods*. John Wiley & Sons. 2008

MC METHOD AND NON-LINEARITIES

- ▶ A quantity $\mathcal{P}(t)$ is evaluated with MCM

$$\mathcal{P}(t) = \int_{\mathcal{D}_X} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times \hat{w}(\mathbf{x})$$

- ▶ We estimate a quantity \mathcal{A} with a conversion function f_c :

$$\mathcal{A}(t) = f_c(\mathcal{P}(t))$$

- ▶ We estimate an averaged quantity $\langle \mathcal{A} \rangle$

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times f_c(\mathcal{P}(t))$$

MC METHOD AND NON-LINEARITIES

- ▶ A quantity $\mathcal{P}(t)$ is evaluated with MCM

$$\mathcal{P}(t) = \int_{\mathcal{D}_X} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times \hat{w}(\mathbf{x})$$

- ▶ We estimate a quantity \mathcal{A} with a conversion function f_c :

$$\mathcal{A}(t) = f_c(\mathcal{P}(t))$$

- ▶ We estimate an averaged quantity $\langle \mathcal{A} \rangle$

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times f_c(\mathcal{P}(t))$$

- ▶ If f_c is **linear** $f_c = k \times (\mathcal{P}(t) + \mathcal{P}_0)$:

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times \int_{\mathcal{D}_X} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times k \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0)$$

MC METHOD AND NON-LINEARITIES

- ▶ A quantity $\mathcal{P}(t)$ is evaluated with MCM

$$\mathcal{P}(t) = \int_{\mathcal{D}_{\mathbf{X}}} p_{\mathbf{X}(t)}(\mathbf{x}) \, d\mathbf{x} \times \hat{w}(\mathbf{x})$$

- ▶ We estimate a quantity \mathcal{A} with a conversion function f_c :

$$\mathcal{A}(t) = f_c(\mathcal{P}(t))$$

- ▶ We estimate an averaged quantity $\langle \mathcal{A} \rangle$

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) \, dt \times f_c(\mathcal{P}(t))$$

- ▶ If f_c is **non-linear** $f_c = k \times (\mathcal{P}(t) + \mathcal{P}_0)^2$:

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) \, dt \times k \times \left[\int_{\mathcal{D}_{\mathbf{X}}} p_{\mathbf{X}(t)}(\mathbf{x}) \, d\mathbf{x} \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0) \right]^2$$

MC METHOD AND NON-LINEARITIES

- ▶ A quantity $\mathcal{P}(t)$ is evaluated with MCM

$$\mathcal{P}(t) = \int_{\mathcal{D}_{\mathbf{X}}} p_{\mathbf{X}(t)}(\mathbf{x}) \, d\mathbf{x} \times \hat{w}(\mathbf{x})$$

- ▶ We estimate a quantity \mathcal{A} with a conversion function f_c :

$$\mathcal{A}(t) = f_c(\mathcal{P}(t))$$

- ▶ We estimate an averaged quantity $\langle \mathcal{A} \rangle$

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) \, dt \times f_c(\mathcal{P}(t))$$

- ▶ If f_c is **non-linear** $f_c = k \times (\mathcal{P}(t) + \mathcal{P}_0)^2$:

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) \, dt \times k \times \left[\int_{\mathcal{D}_{\mathbf{X}}} p_{\mathbf{X}(t)}(\mathbf{x}) \, d\mathbf{x} \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0) \right]^2$$

MC METHOD AND NON-LINEARITIES

- ▶ A quantity $\mathcal{P}(t)$ is evaluated with MCM

$$\mathcal{P}(t) = \int_{\mathcal{D}_X} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times \hat{w}(\mathbf{x})$$

- ▶ We estimate a quantity \mathcal{A} with a conversion function f_c :

$$\mathcal{A}(t) = f_c(\mathcal{P}(t))$$

- ▶ We estimate an averaged quantity $\langle \mathcal{A} \rangle$

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times f_c(\mathcal{P}(t))$$

- ▶ If f_c is **non-linear** $f_c = k \times (\mathcal{P}(t) + \mathcal{P}_0)^2$:

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times k \times \underbrace{\left[\int_{\mathcal{D}_X} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times k \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0) \right]^2}_{\mathcal{A}(t)}$$

MC METHOD AND NON-LINEARITIES

- ▶ A quantity $\mathcal{P}(t)$ is evaluated with MCM

$$\mathcal{P}(t) = \int_{\mathcal{D}_X} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times \hat{w}(\mathbf{x})$$

- ▶ We estimate a quantity \mathcal{A} with a conversion function f_c :

$$\mathcal{A}(t) = f_c(\mathcal{P}(t))$$

- ▶ We estimate an averaged quantity $\langle \mathcal{A} \rangle$

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times f_c(\mathcal{P}(t))$$

- ▶ If f_c is **non-linear** $f_c = k \times (\mathcal{P}(t) + \mathcal{P}_0)^2$: **n^2 MC realizations**

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times k \times \underbrace{\left[\int_{\mathcal{D}_X} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times k \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0) \right]^2}_{\mathcal{A}(t)}$$

MC METHOD AND NON-LINEARITIES

- ▶ Introduction of two independent random variables X_1 et X_2

$$\left[\int_{\mathcal{D}_{\mathbf{x}}} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0) \right]^2 = \int_{\mathcal{D}_{\mathbf{x}_1}} p_{\mathbf{X}_1(t)}(\mathbf{x}_1) d\mathbf{x}_1 \times (\hat{w}(\mathbf{x}_1) + \mathcal{P}_0) \times \int_{\mathcal{D}_{\mathbf{x}_2}} p_{\mathbf{X}_2(t)}(\mathbf{x}_2) d\mathbf{x}_2 \times (\hat{w}(\mathbf{x}_2) + \mathcal{P}_0)$$

- ▶ \Rightarrow rewriting of $\langle \mathcal{A} \rangle$:

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times \int_{\mathcal{D}_{\mathbf{x}_1}} p_{\mathbf{X}_1(t)}(\mathbf{x}_1) d\mathbf{x}_1 \times \int_{\mathcal{D}_{\mathbf{x}_2}} p_{\mathbf{X}_2(t)}(\mathbf{x}_2) d\mathbf{x}_2 \times \hat{w}(\mathbf{x}_1, \mathbf{x}_2)$$

MC METHOD AND NON-LINEARITIES

- ▶ Introduction of two independent random variables X_1 et X_2

$$\left[\int_{\mathcal{D}_{\mathbf{x}}} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0) \right]^2 = \int_{\mathcal{D}_{\mathbf{x}_1}} p_{\mathbf{X}_1(t)}(\mathbf{x}_1) d\mathbf{x}_1 \times (\hat{w}(\mathbf{x}_1) + \mathcal{P}_0) \times \int_{\mathcal{D}_{\mathbf{x}_2}} p_{\mathbf{X}_2(t)}(\mathbf{x}_2) d\mathbf{x}_2 \times (\hat{w}(\mathbf{x}_2) + \mathcal{P}_0)$$

- ▶ \Rightarrow rewriting of $\langle \mathcal{A} \rangle$: **$2 \times n$ MC realizations**

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times \int_{\mathcal{D}_{\mathbf{x}_1}} p_{\mathbf{X}_1(t)}(\mathbf{x}_1) d\mathbf{x}_1 \times \int_{\mathcal{D}_{\mathbf{x}_2}} p_{\mathbf{X}_2(t)}(\mathbf{x}_2) d\mathbf{x}_2 \times \hat{w}(\mathbf{x}_1, \mathbf{x}_2)$$

MC METHOD AND NON-LINEARITIES

- ▶ Introduction of two independent random variables X_1 et X_2

$$\left[\int_{\mathcal{D}_{\mathbf{x}}} p_{\mathbf{X}(t)}(\mathbf{x}) d\mathbf{x} \times (\hat{w}(\mathbf{x}) + \mathcal{P}_0) \right]^2 = \int_{\mathcal{D}_{\mathbf{x}_1}} p_{\mathbf{X}_1(t)}(\mathbf{x}_1) d\mathbf{x}_1 \times (\hat{w}(\mathbf{x}_1) + \mathcal{P}_0) \times \int_{\mathcal{D}_{\mathbf{x}_2}} p_{\mathbf{X}_2(t)}(\mathbf{x}_2) d\mathbf{x}_2 \times (\hat{w}(\mathbf{x}_2) + \mathcal{P}_0)$$

- ▶ \Rightarrow rewriting of $\langle \mathcal{A} \rangle$:

$$\langle \mathcal{A} \rangle = \int_{\tau} p_{\tau}(t) dt \times \int_{\mathcal{D}_{\mathbf{x}_1}} p_{\mathbf{X}_1(t)}(\mathbf{x}_1) d\mathbf{x}_1 \times \int_{\mathcal{D}_{\mathbf{x}_2}} p_{\mathbf{X}_2(t)}(\mathbf{x}_2) d\mathbf{x}_2 \times \hat{w}(\mathbf{x}_1, \mathbf{x}_2)$$

- ▶ Could be generalized with **Taylor series expansion**⁸

⁸I. Dauchet. "Analyse radiative des photobioréacteurs". PhD thesis. Université Blaise Pascal Clermont-Ferrand II. 2012

STATISTICAL MODELLING OF ENERGY CONVERSION EFFICIENCY

- ▶ $\eta_r(t) = f(P_{th}(t))$ is decomposed with Taylor series expansion around P_{th0}

$$\eta_r(t) = f(P_{th}(t)) = f(P_{th0}) + \frac{f'(P_{th0})}{1!} (P_{th}(t) - P_{th0}) + \frac{f^{(2)}(P_{th0})}{2!} (P_{th}(t) - P_{th0})^2 + \dots + \frac{f^{(n)}(P_{th0})}{n!} (P_{th}(t) - P_{th0})^n + R_n(P_{th}(t))$$

$$\langle \eta_r \rangle = \int_{Lifetime} \eta_r(t) dt$$

- ▶ The expansion is stopped \Rightarrow Bernoulli process \Rightarrow no statistical bias introduced
 - ▶ A probability \mathcal{P}_i based on $P_{th}(t)$ is introduced
 - ▶ A random number r_i is sampled in $[0; 1]$
 - ▶ If $r_i < \mathcal{P}_i$, the Taylor expansion serie continue to at degree $i + 1$
 - ▶ Else, the Taylor expansion serie is stopped at degree i

OUTLINES

Modelling of a solar reactor plant

Estimation of the lifetime energy conversion efficiency

Monte Carlo modelling

Simulation results

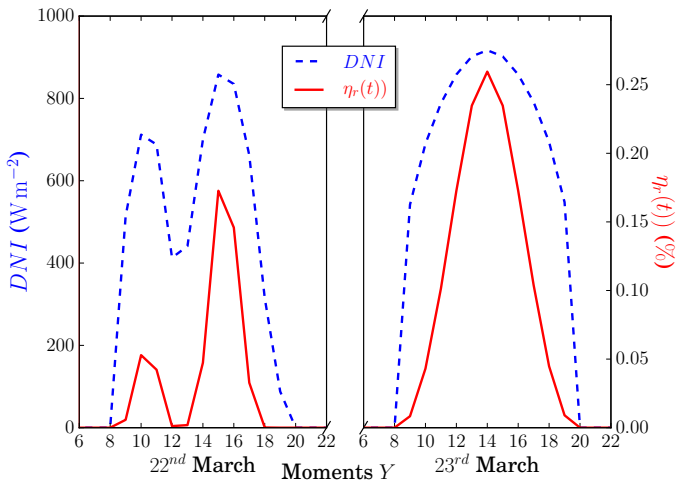
Conclusion and Outlook

CASE STUDY

- ▶ Use an exemple presented by L. Schunk, W. Lipiński, and A. Steinfeld⁹ : a 1 MW reactor
- ▶ with a solar plant which delivers at most the nominal power

⁹L. 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". In: *Chemical Engineering Journal* 150.2–3 (2009), pp. 502–508

SIMULATION RESULTS



Instantaneous energy conversion efficiency estimation

Results

Values

Instantaneous energy conversion efficiency η_r ¹⁰	54 %
Instantaneous energy conversion efficiency η_r	40,2 %

¹⁰L. 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". In: *Chemical Engineering Journal* 150.2-3 (2009), pp. 502-508

Instantaneous energy conversion efficiency estimation

Results	Values
Instantaneous energy conversion efficiency η_r ¹⁰	54 %
Instantaneous energy conversion efficiency η_r	40,2 %

with MCM

Yearly averaged energy conversion efficiency $\langle \eta_r \rangle = 4,8 \% \cdot \text{yr}^{-1}$

¹⁰L. 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". In: *Chemical Engineering Journal* 150.2–3 (2009), pp. 502–508

DEPENDANCE OF THE SOLAR RESOURCE

- ▶ The yearly averaged conversion efficiency is dependent to the solar resource

Location	conversion eff.
Sevilla	$4,8 \% \cdot \text{yr}^{-1} \pm 0.00026$
Casablanca	$5,5 \% \cdot \text{yr}^{-1} \pm 0.00024$
Albuquerque	$9 \% \cdot \text{yr}^{-1} \pm 0.00042$

OUTLINES

Modelling of a solar reactor plant

Estimation of the lifetime energy conversion efficiency

Monte Carlo modelling

Simulation results

Conclusion and Outlook

CONCLUSION

- ▶ We propose a method to estimate nonlinear efficiency with MC method
- ▶ All MC advantages could be applied to complex systems with nonlinear outputs
 - ▶ Solar plant
 - ▶ Wave scattering
 - ▶ Biomass production
 - ▶ Atmospheric radiative transfer
 - ▶ ...

- ▶ Modelling with MCM of coupled heat transfer of the reactor: 2 PhD just started on a statistical approach to deal with coupled heat transfer in complex geometries
- ▶ Take into account the evolution of the solar resource \Rightarrow coupling with General Circulation Model (GCM)

Thank you for your attention