SFERA-III

Solar Facilities for the European Research Area

4th Doctoral Colloquium
Cologne, Germany, September 11th-13th 2023

Development of a Redox Material Assembly for Solar Thermochemical Fuel Production

Louis Thomas, DLR Institute of Future Fuels
louis.thomas@dlr.de

NETWORKING

Examiner: Prof. Dr. Christian Sattler
Supervisor: Dr.-Ing. Stefan Brendelberger

THIS PROJECT HAS RECEIVED FUNDING FROM THE EUROPEAN UNION'S HORIZON 2020 RESEARCH AND INNOVATION PROGRAMME UNDER GRANT AGREEMENT NO **823802**

Overview

Solar Fuel Production
Thermochemical Redox Cycle


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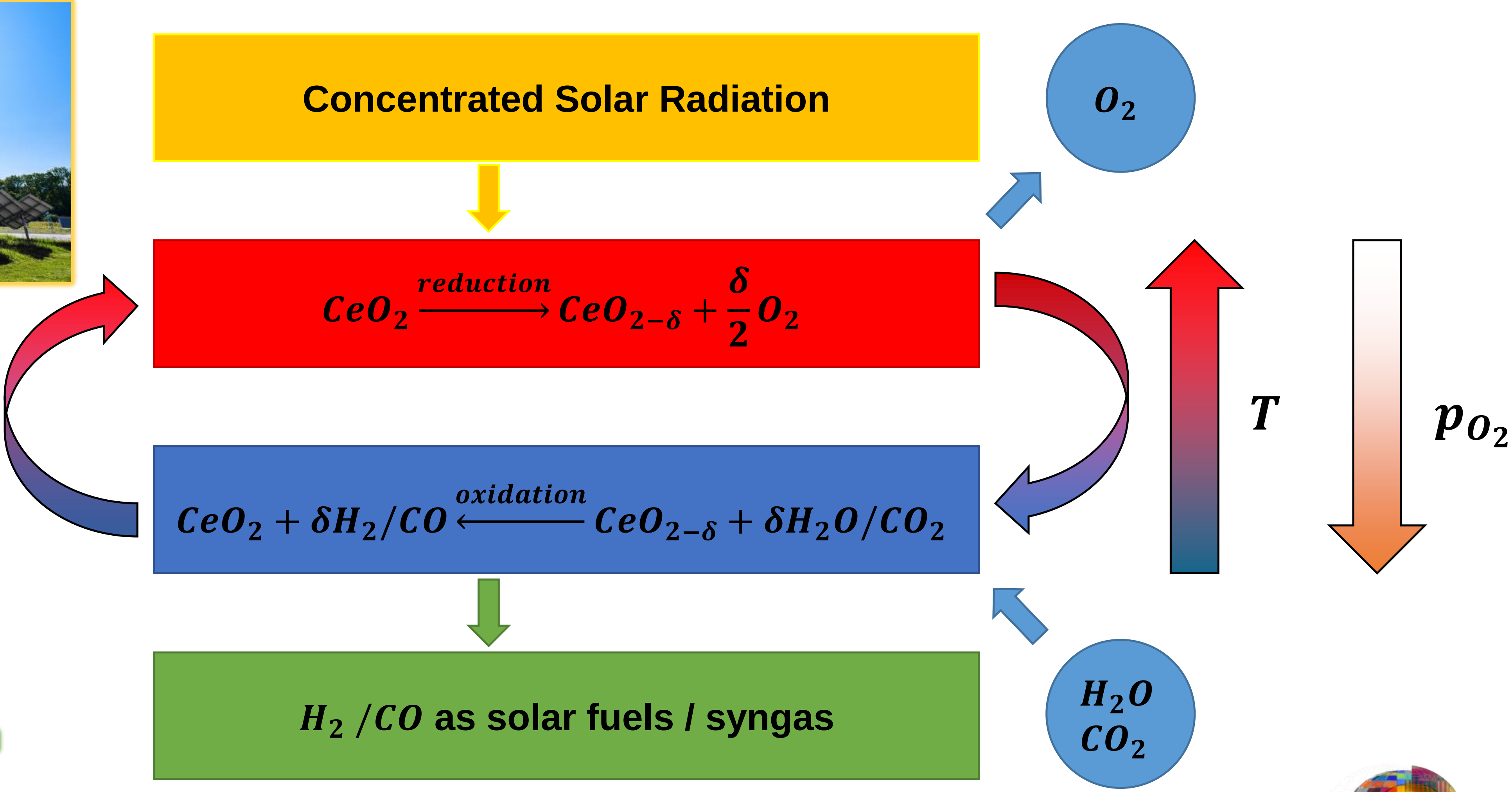
Concentrated Solar Radiation

$$CeO_2 \xrightarrow{reduction} CeO_{2-\delta} + \frac{\delta}{2} O_2$$

$$CeO_2 + \delta H_2/CO \xleftarrow{oxidation} CeO_{2-\delta} + \delta H_2O/CO_2$$

H_2 /CO as solar fuels / syngas

Louis Thomas

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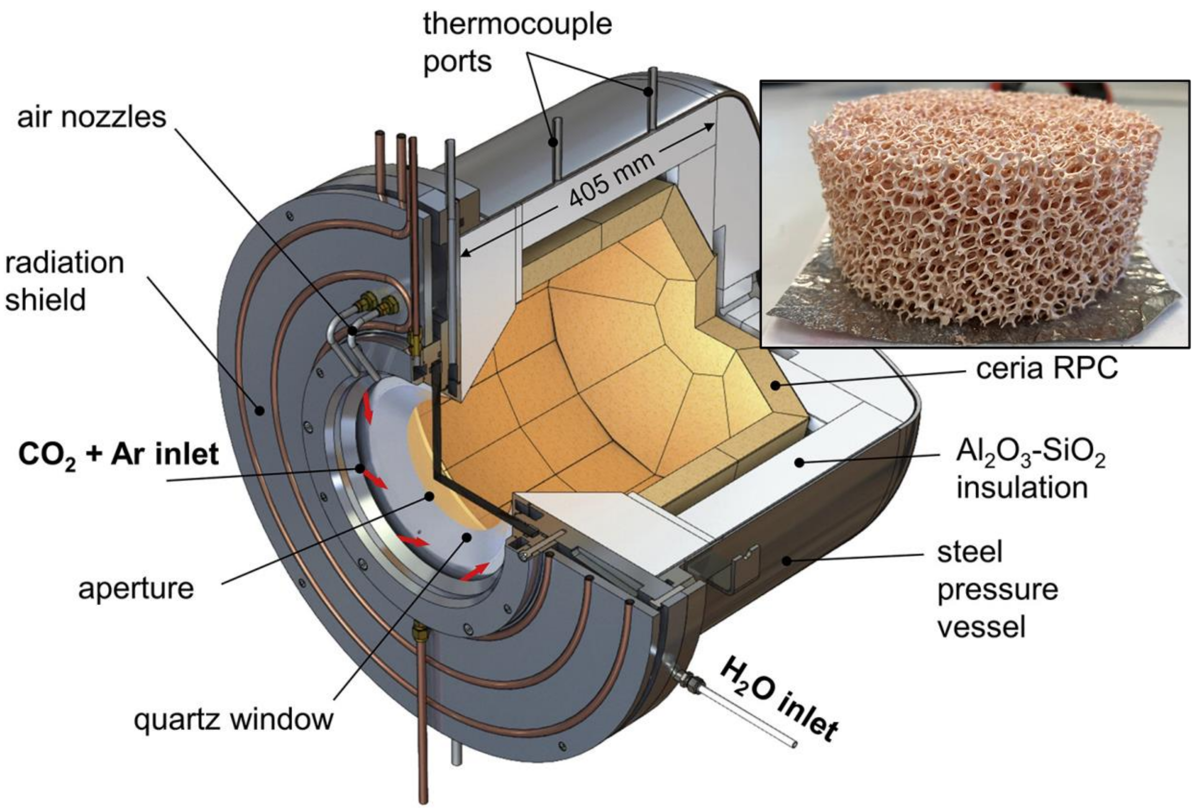
State of the Art

Reactor Concept and Redox Material

- Redox material: Ceria RPC (reticulated porous ceramic) structure
- RPC blocks mounted at reactor cavity walls
- Batch operation with temperature / pressure swing between reduction and oxidation step

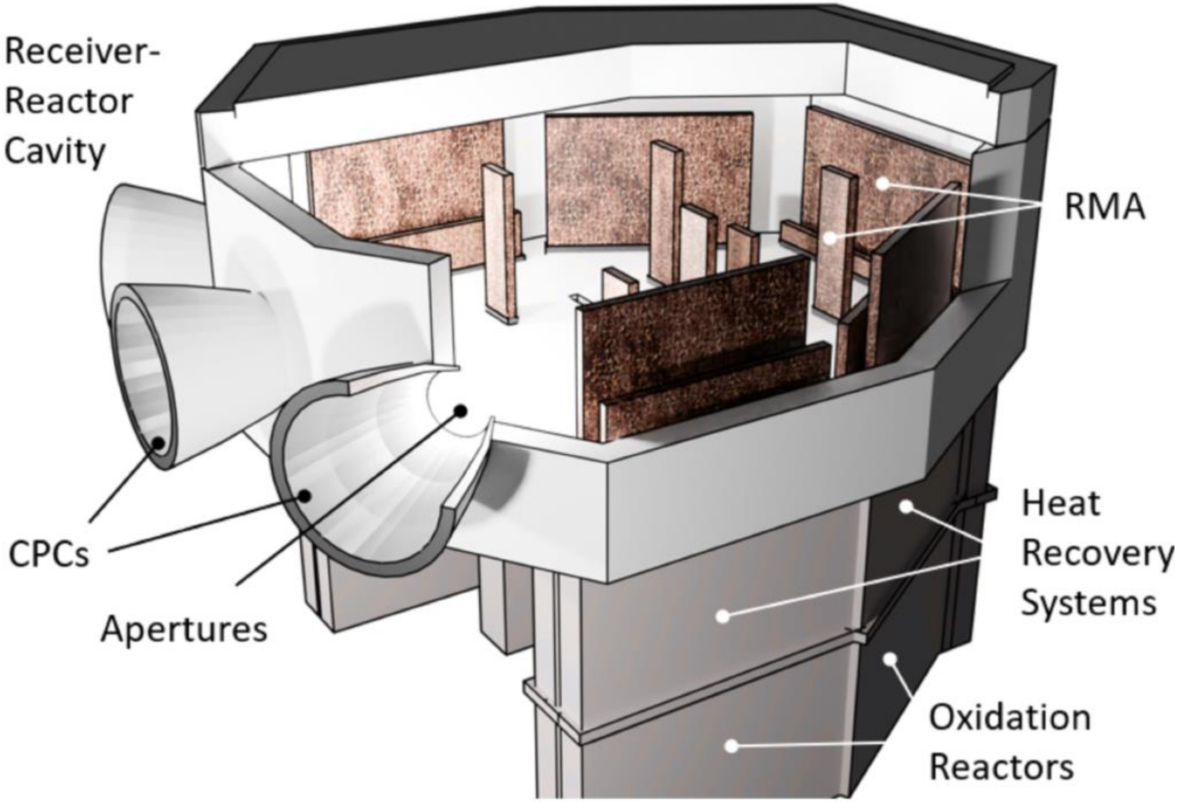


S. Zoller, E. Koepf, D. Nizamian, M. Stephan, A. Patané, P. Haueter, M. Romero, J. González-Aguilar, D. Lieftink, E. de Wit, S. Brendelberger, A. Sizmann, and A. Steinfeld, Joule 6, 1606 (2022).

R2Mx Reactor

Reactor Features of MW-Scale Vision

- Separate reduction and oxidation reactor cavities
- Receiver reactor cavity stays at high temperature, continuous on-sun operation
- Multiple movable **Redox Material Assembly (RMA)** units

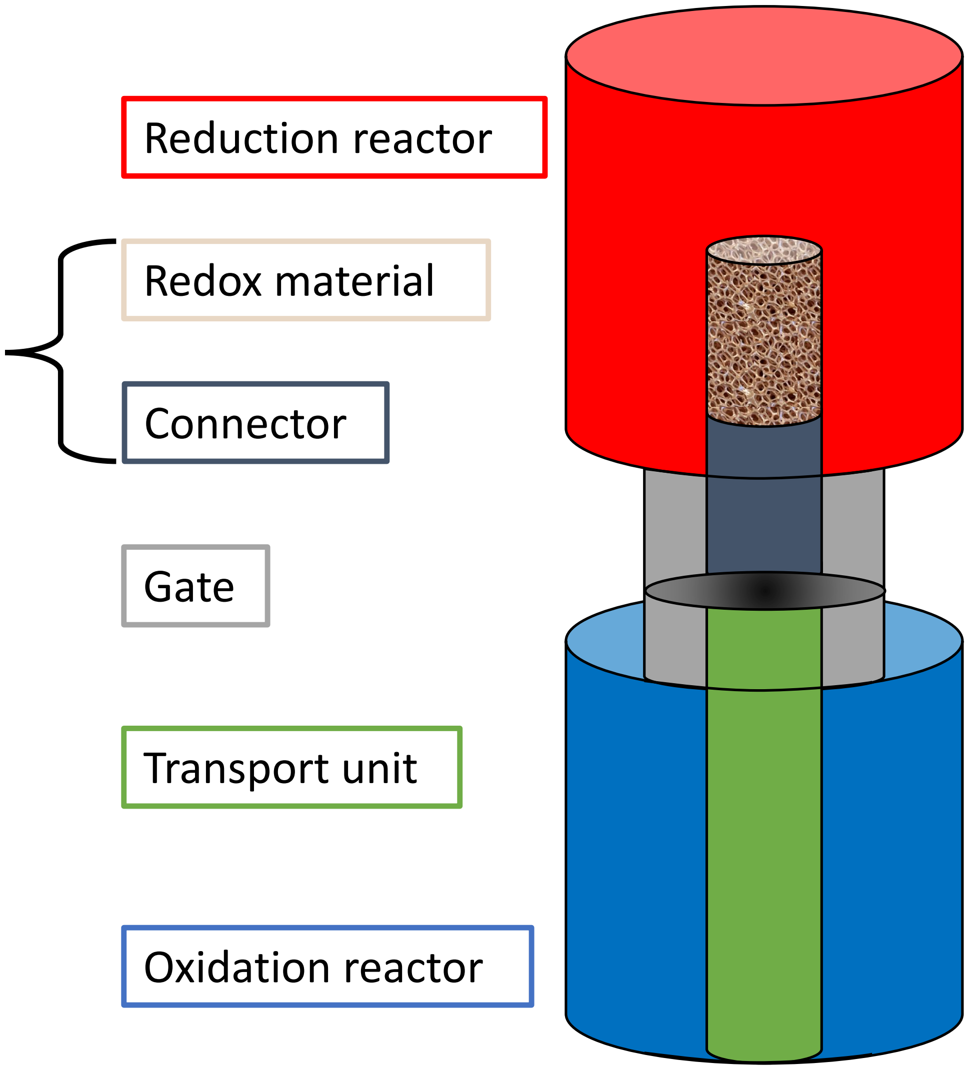


S. Brendelberger, P. Holzemer-Zerhusen, E. Vega Puga, M. Roeb, and C. Sattler, Solar Energy 235, 118 (2022).

R2Mx Reactor

Proof-of-Concept Test Rig

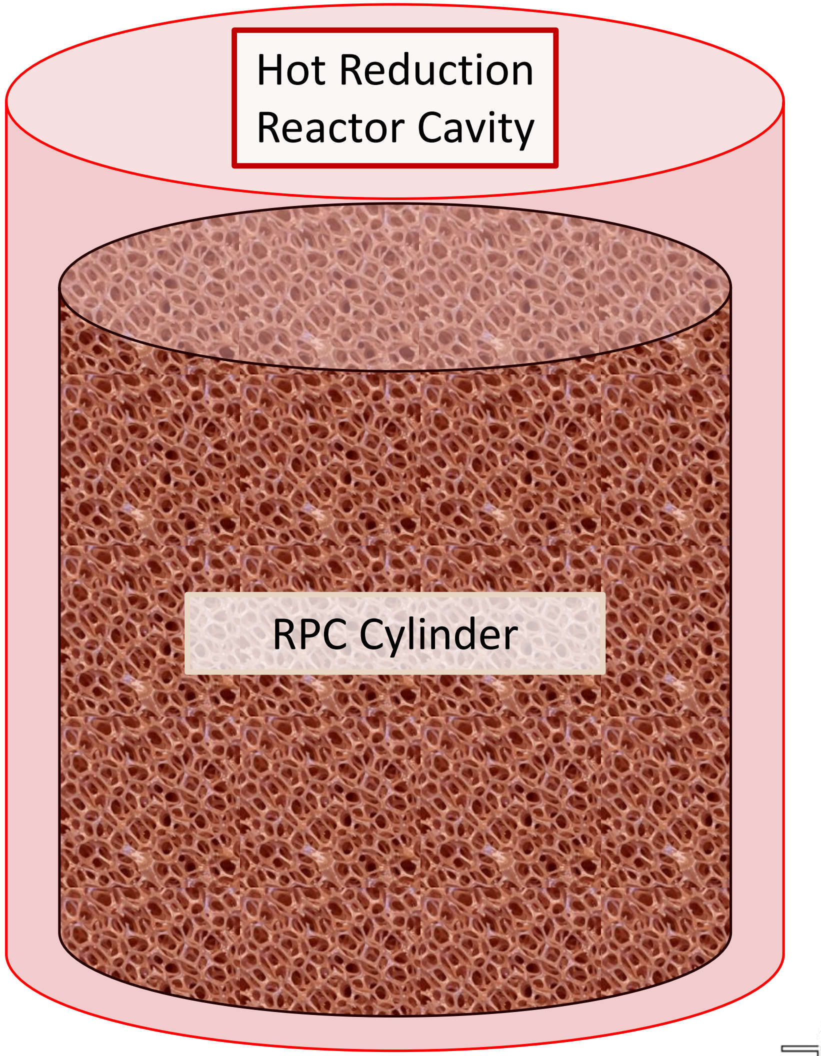
- Separate reactor cavities with **cylindrical shape** for practical implementation and manufacturing
- **Cylindrical Redox Material Assembly (RMA)**, which is moved between reduction and oxidation reactor via linear transport unit
- Uniform thermal irradiation of RPC cylinder via electrical heating (no solar interface)



Modeling Goal

Radiation Attenuation and Absorption in RPC Cylinder

- Understanding the behavior of an RPC cylinder inside the R2Mx test-rig
- Intensity attenuation and absorption characteristics in radial direction
- Compare to flat RPC plate and collimated irradiation



Intensity Attenuation of Radiation

In $CeO_{2-\delta}$ RPC Structure

Intensity attenuation in $CeO_{2-\delta}$ RPC structure (Beer-Lambert-Law):

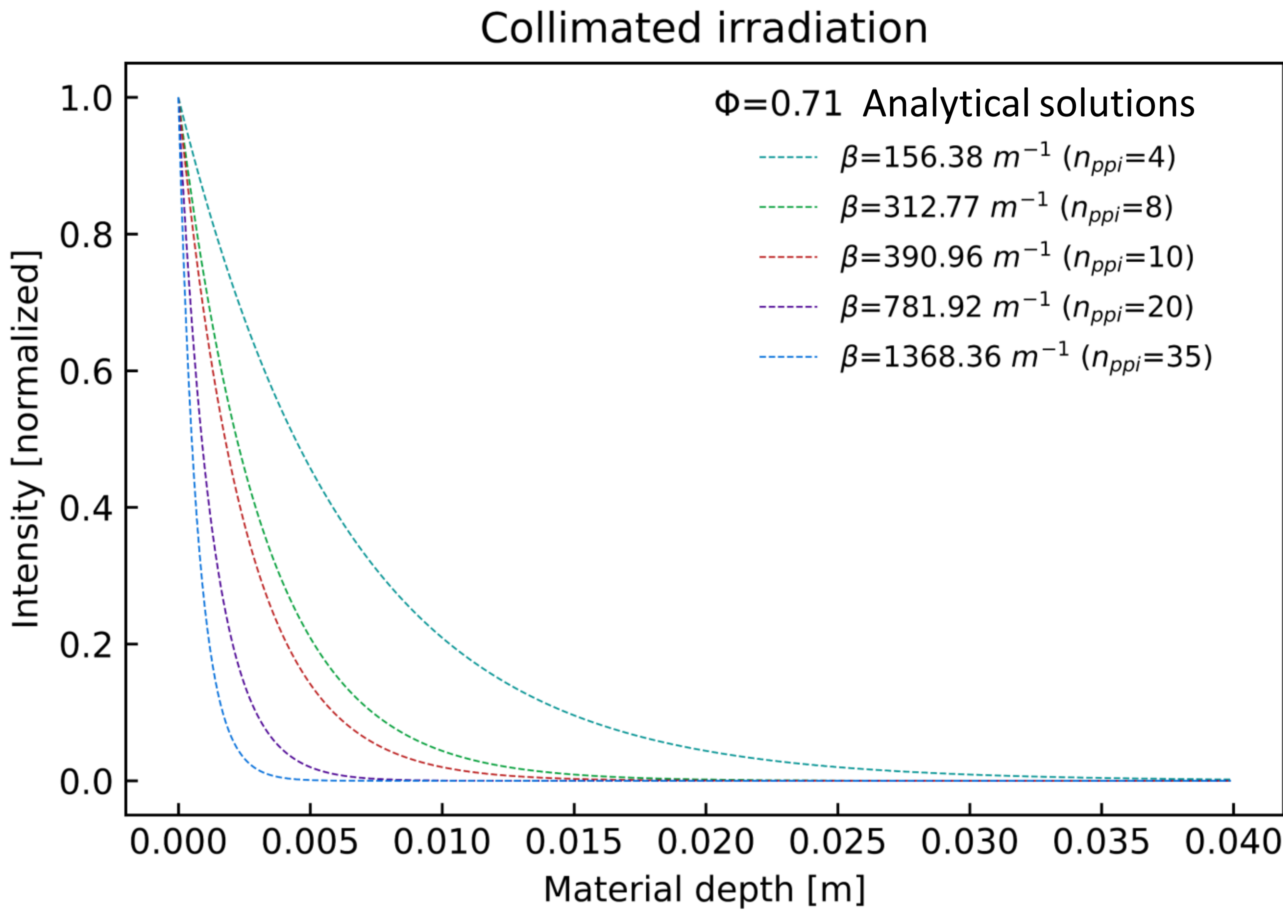
$$\frac{I(x)}{I_0} = \exp(-\beta x)$$

Extinction coefficient: $\beta \propto \frac{\phi^2}{d_m}$ [1]

Mean pore diameter: $d_m \propto \frac{\phi}{n_{ppi}}$ [1]

RPC porosity: ϕ

Pores per inch: n_{ppi}



[1] S. Ackermann, M. Takacs, J. Scheffe, and A. Steinfeld, International Journal of Heat and Mass Transfer 107, 439 (2017).

Absorption of Radiation

In $CeO_{2-\delta}$ RPC Structure

Radiation absorption of $CeO_{2-\delta}$ RPC structure:

$$\alpha = 1 - r = \varepsilon$$

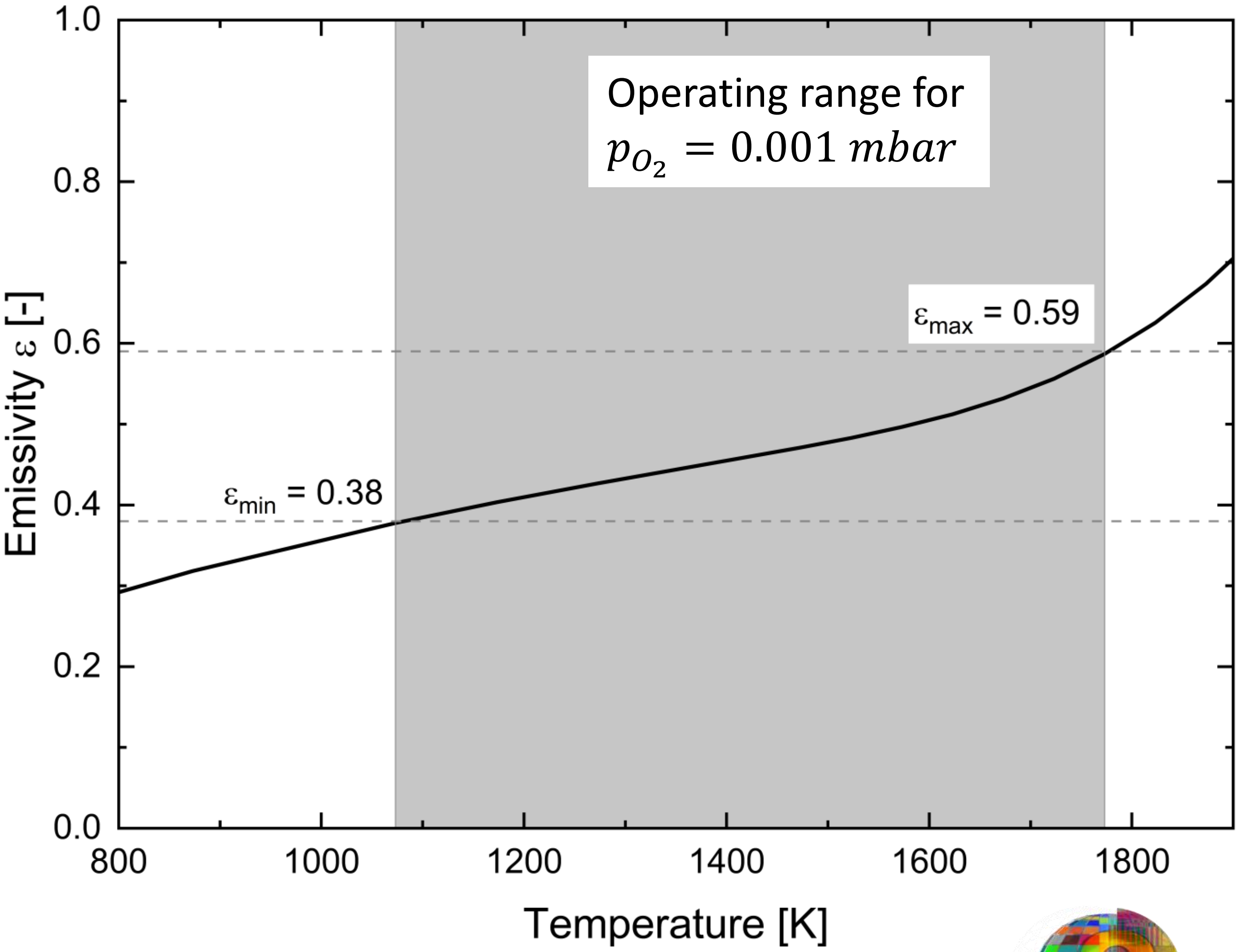
Total hemispherical reflectivity:

$$r_{CeO_{2-\delta}}(\delta, T) = \frac{b}{(\delta+\delta^*)^a} + c * \delta$$ [2]

Reduction extent: $\delta(T, p_{O_2})$

Fitting parameters: $a(T), b(T), c(T)$

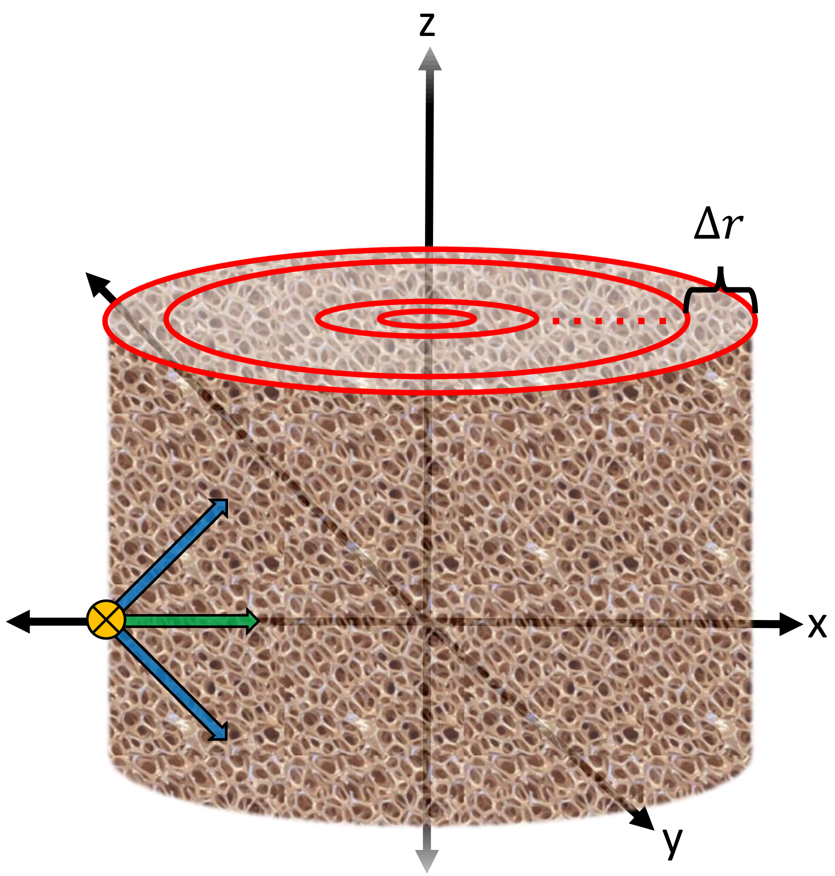
For continuity (at $\delta = 0$): $\delta^* = 10^{-10}$



[2] S. Ackermann and A. Steinfeld, Solar Energy Materials and Solar Cells 159, 167 (2017).

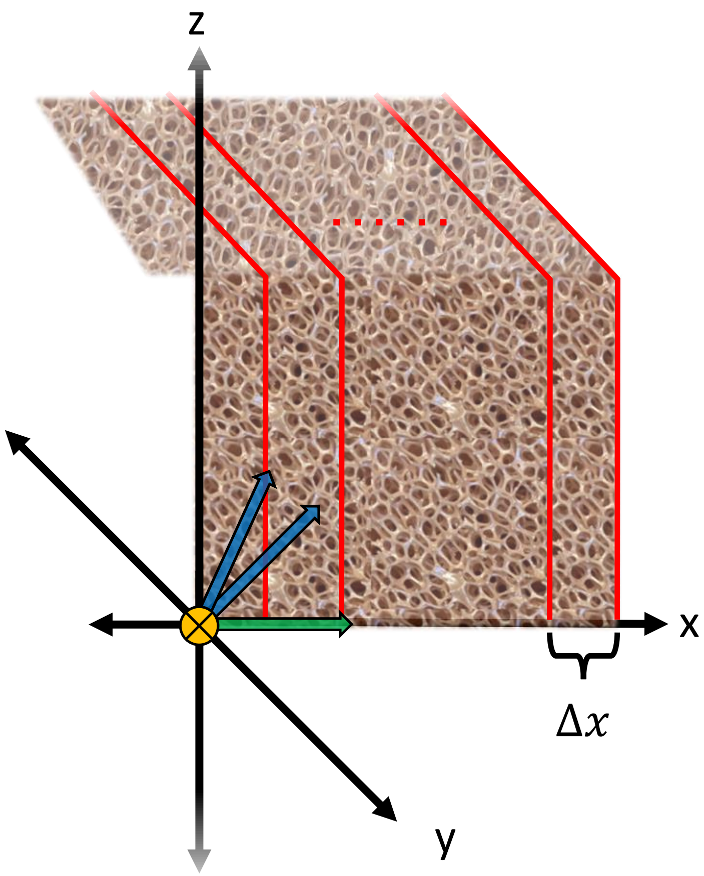
Modeling Approach

RPC Geometry and Irradiation Type

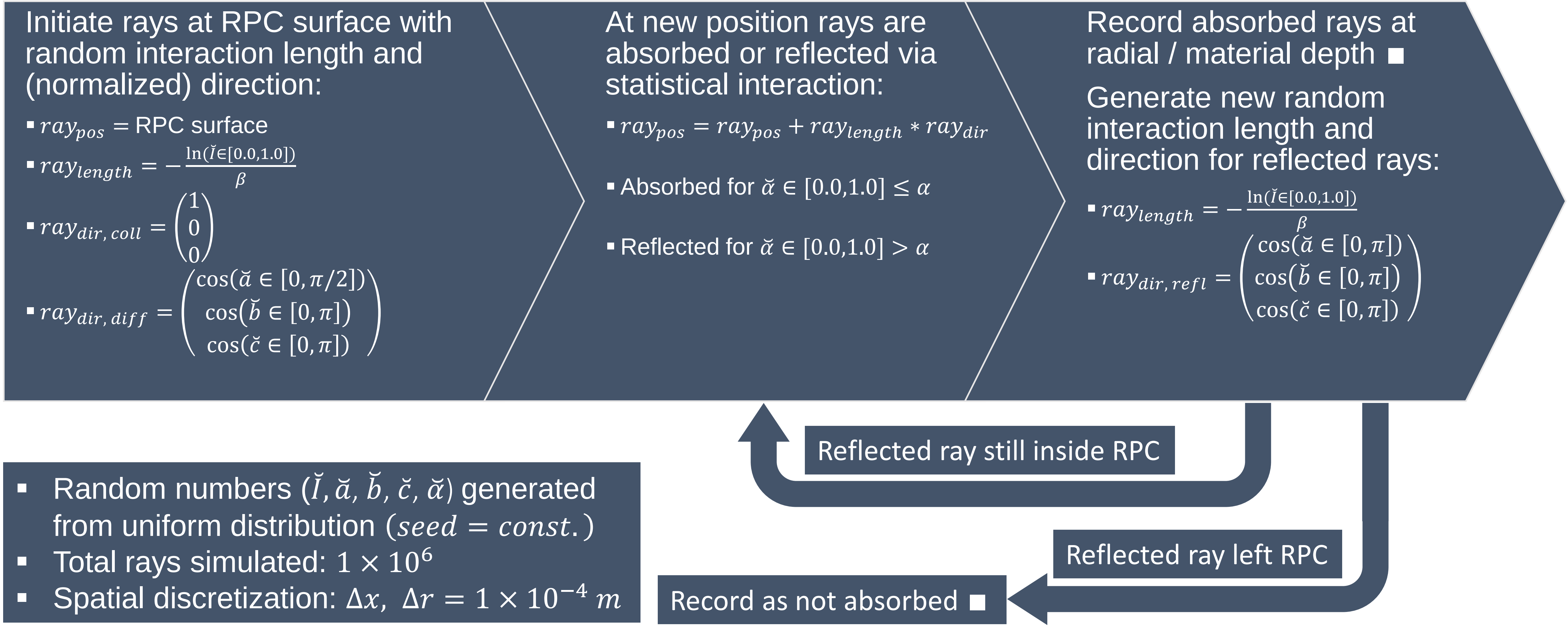


Compare 4 modeling cases:

1. RPC cylinder
   - Collimated irradiation
   - Diffuse irradiation
2. RPC plate
   - Collimated irradiation
   - Diffuse irradiation



Model Implementation
Monte Carlo Simulation (Python)



Initiate rays at RPC surface with random interaction length and (normalized) direction:

- ray_{pos} = RPC surface
- $ray_{length} = -\frac{\ln(\breve{I} \in [0.0,1.0])}{\beta}$
- $ray_{dir,\,coll} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$
- $ray_{dir,\,diff} = \begin{pmatrix} \cos(\breve{a} \in [0,\pi/2]) \\ \cos(\breve{b} \in [0,\pi]) \\ \cos(\check{c} \in [0,\pi]) \end{pmatrix}$

At new position rays are absorbed or reflected via statistical interaction:

- $ray_{pos} = ray_{pos} + ray_{length} * ray_{dir}$
- Absorbed for $\breve{\alpha} \in [0.0,1.0] \leq \alpha$
- Reflected for $\breve{\alpha} \in [0.0,1.0] > \alpha$

Record absorbed rays at radial / material depth ■

Generate new random interaction length and direction for reflected rays:

- $ray_{length} = -\frac{\ln(\breve{I} \in [0.0,1.0])}{\beta}$
- $ray_{dir,\,refl} = \begin{pmatrix} \cos(\breve{a} \in [0,\pi]) \\ \cos(\breve{b} \in [0,\pi]) \\ \cos(\check{c} \in [0,\pi]) \end{pmatrix}$

Reflected ray still inside RPC

Reflected ray left RPC

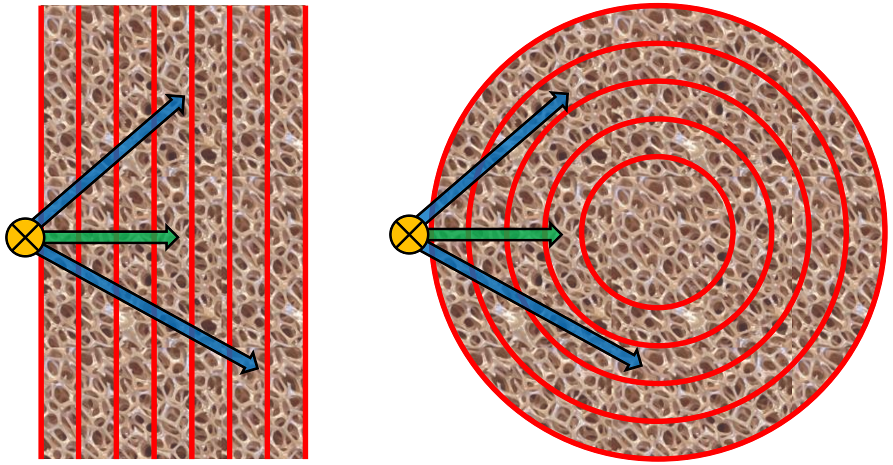
Record as not absorbed ■

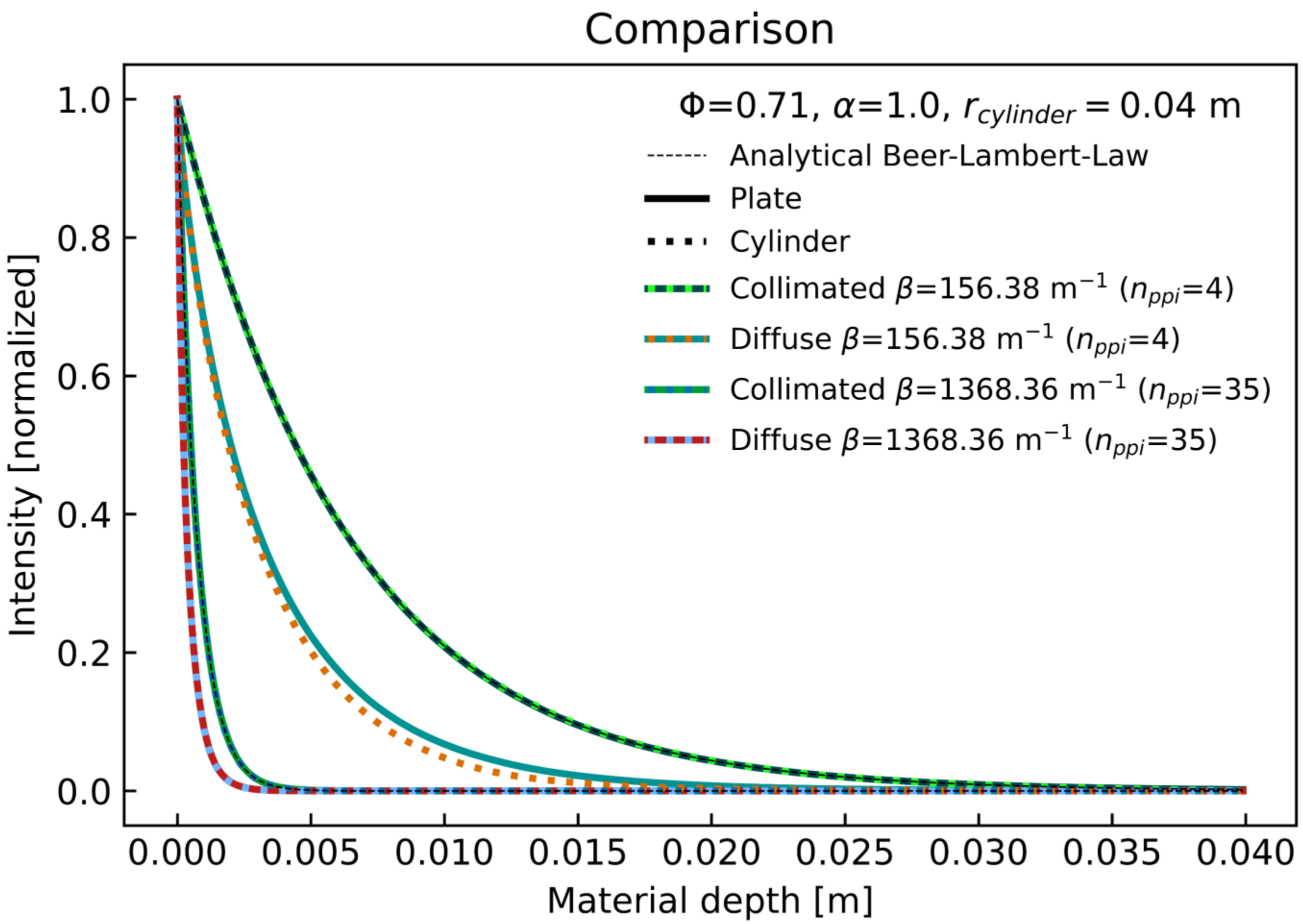
- Random numbers $(\breve{I}, \breve{a}, \breve{b}, \check{c}, \breve{\alpha})$ generated from uniform distribution $(seed = const.)$
- Total rays simulated: 1×10^6
- Spatial discretization: $\Delta x,\ \Delta r = 1 \times 10^{-4}\ m$

Modeling Results: Intensity attenuation

Variation of Extinction Coefficient β (n_{ppi} variation)

- Intensity attenuation for diffuse irradiation stronger due to steep incident angles
- For high extinction coefficients differences between collimated and diffuse irradiation decrease

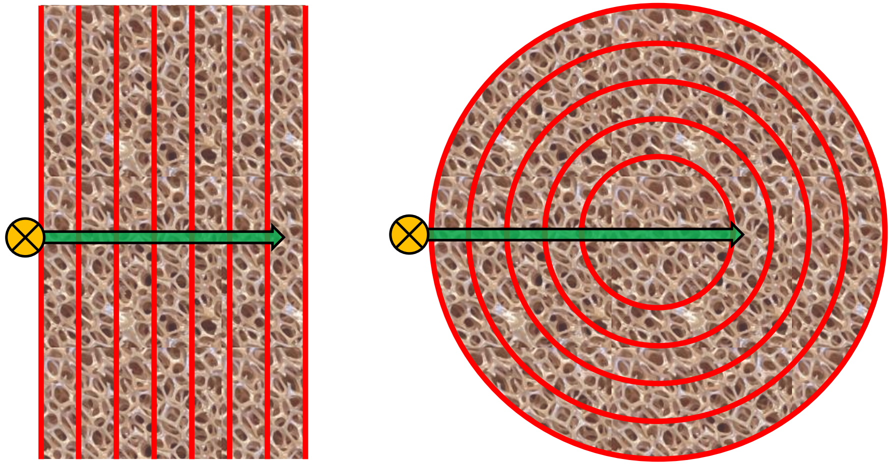


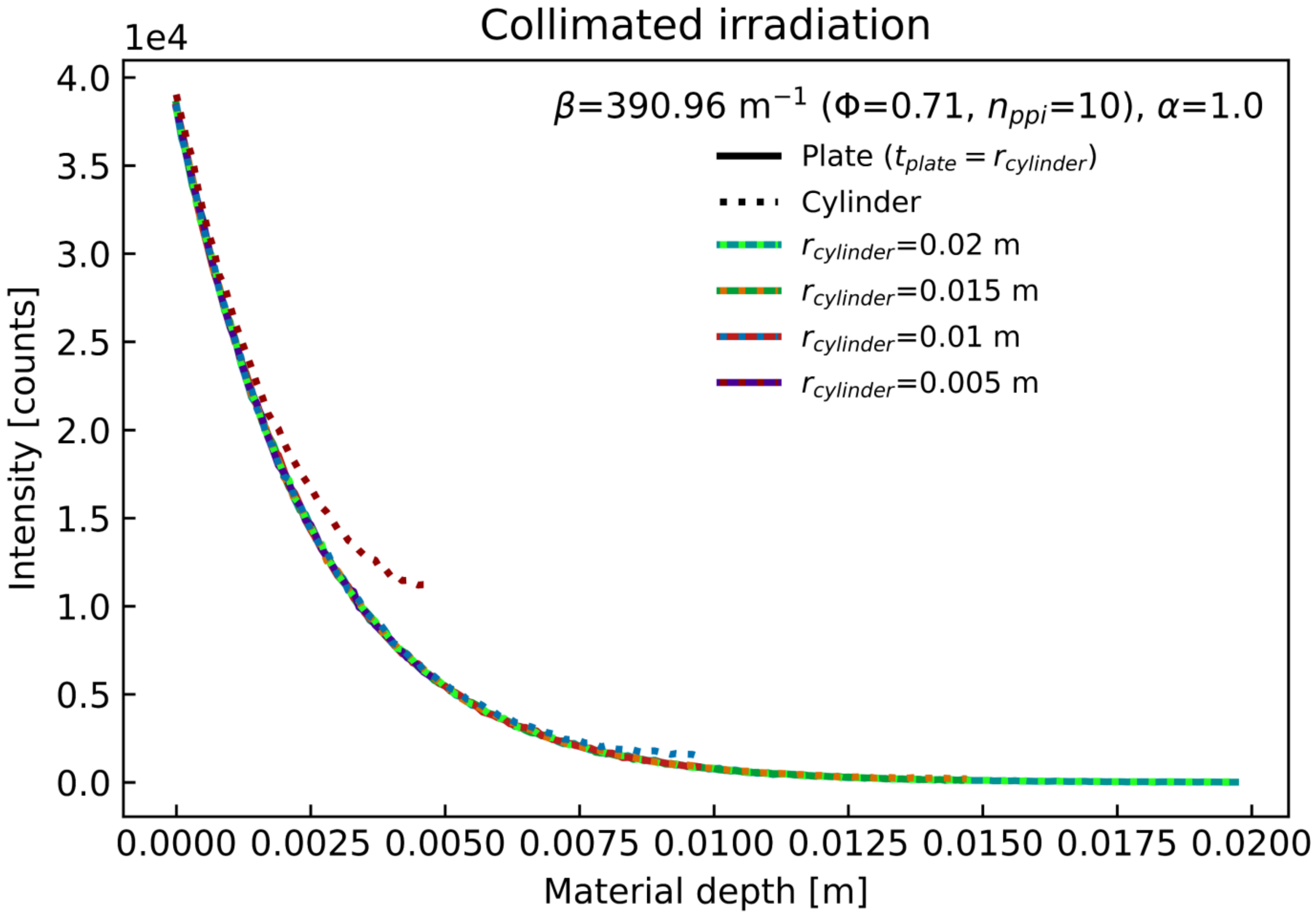


Modeling Results: Intensity attenuation

Variation of Cylinder Radius / Material Thickness

- For smaller cylinder $(r_{cylinder} \leq 0.01\ m)$ rays reach inner radial segments in 2nd cylinder half, resulting in increased intensity counts in inner segments

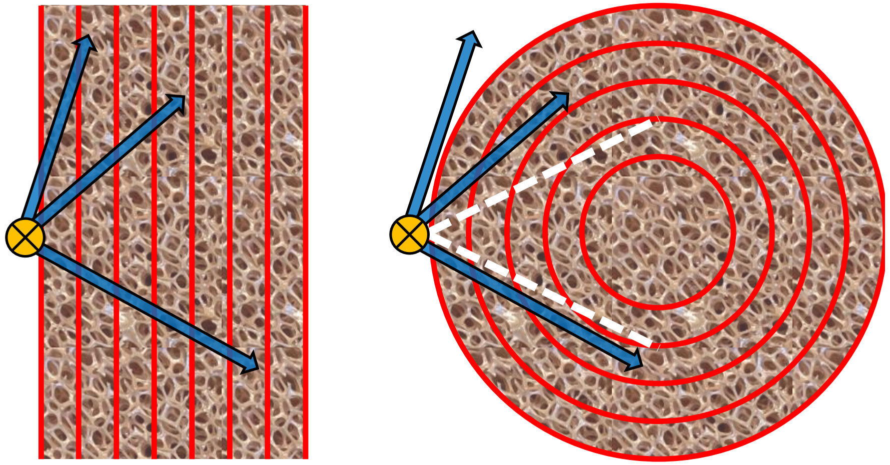


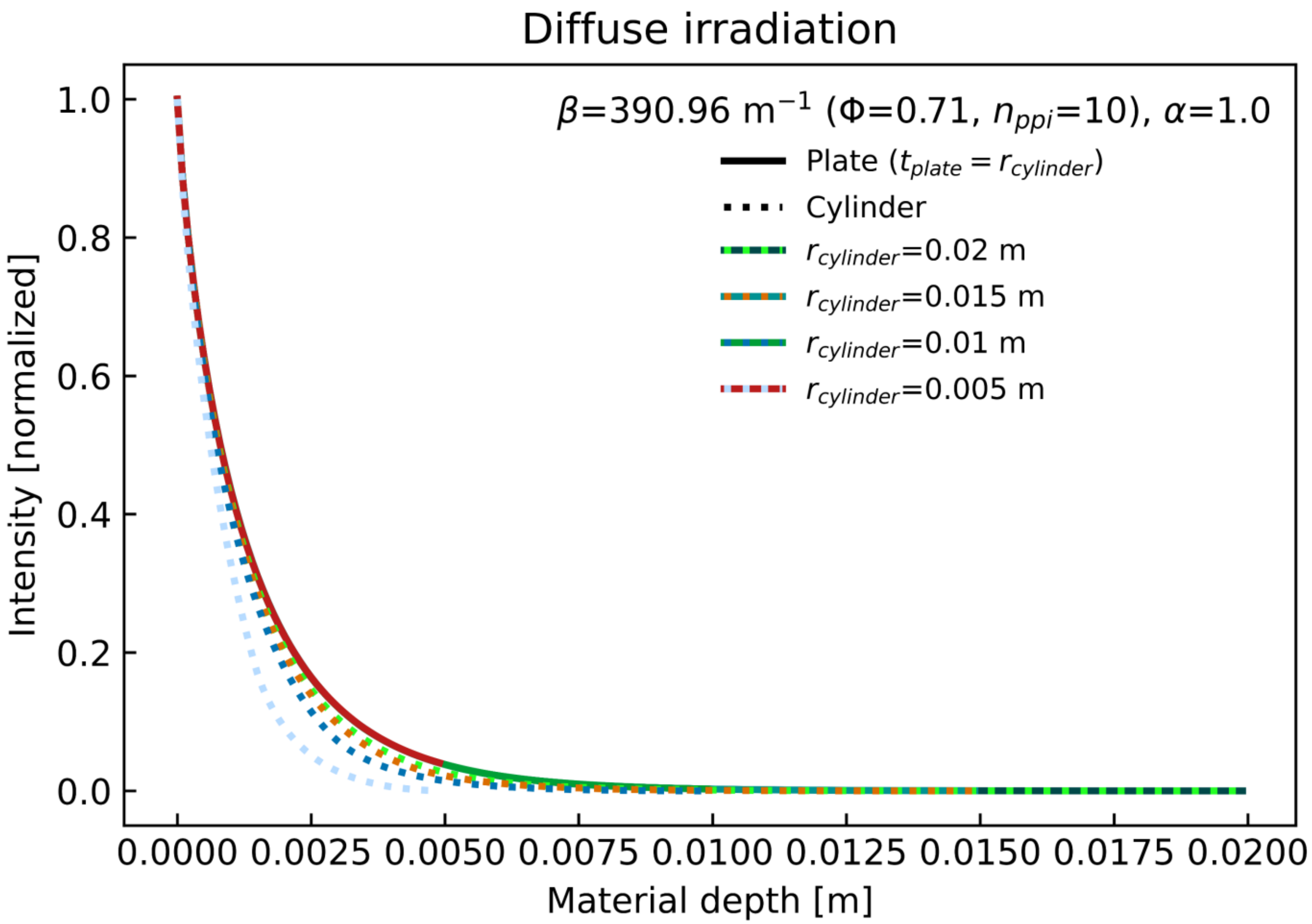


Modeling Results: Intensity attenuation

Variation of Cylinder Radius / Material Thickness

- For smaller cylinder radii the range of incident angles for rays reaching inner radial segments decreases
- For cylinder a larger fraction of total volume is located in outer segments compared to plate





Summary and Outlook

- Intensity attenuation related to parameter variation of RPC cylinder:
  - Diffuse irradiation is stronger attenuated in RPC structure compared to collimated irradiation
  - Cylinder with $r_{cylinder} \geq 0.02\ \mathrm{m}$ exhibits intensity attenuation similar to plate
  - Cylinder with $r_{cylinder} \leq 0.015\ \mathrm{m}$ intensity attenuation is influenced by radial symmetry

- Outlook on further modeling tasks:
  - Include additional technical reactor boundary conditions into model (e.g. distance between hot cavity and RPC cylinder)
  - Set up thermal model of cylindrical RMA unit inside R2Mx reactor

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WP1 Capacity building and training activities
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Backup Slides

NETWORKING

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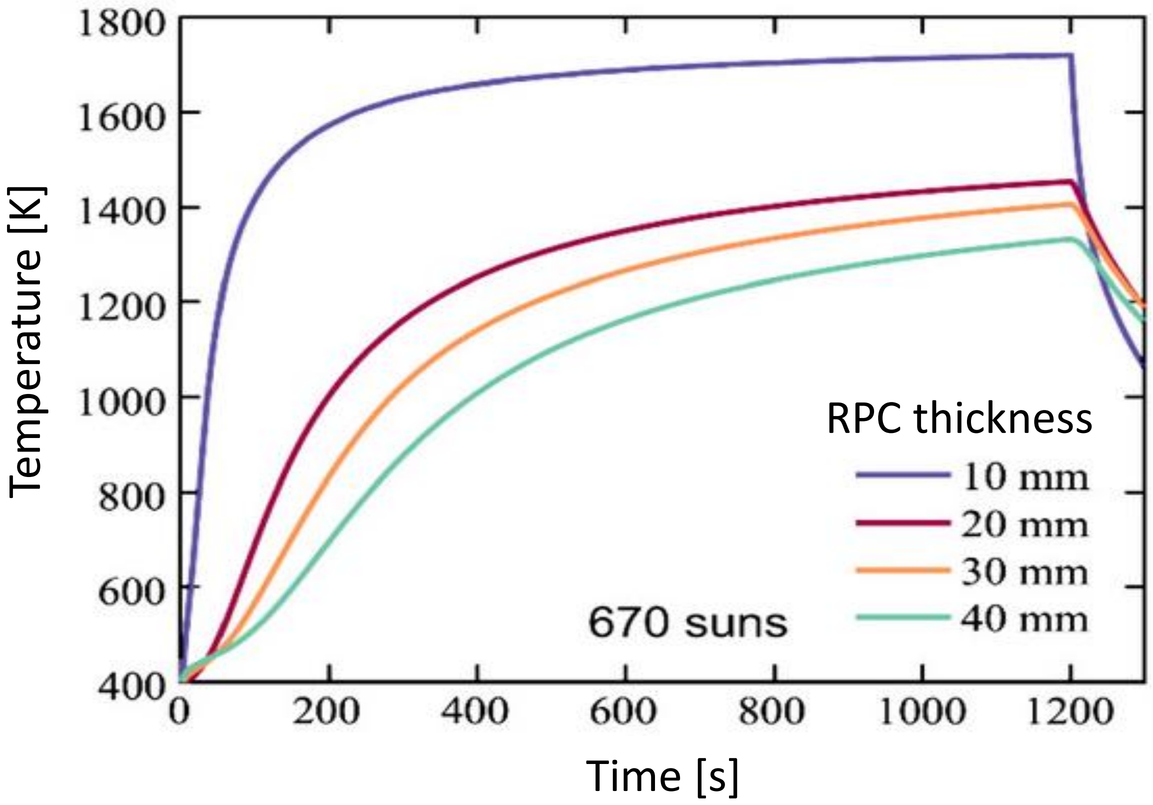
Challenges

Reactor Design / Operation and RPC Structure

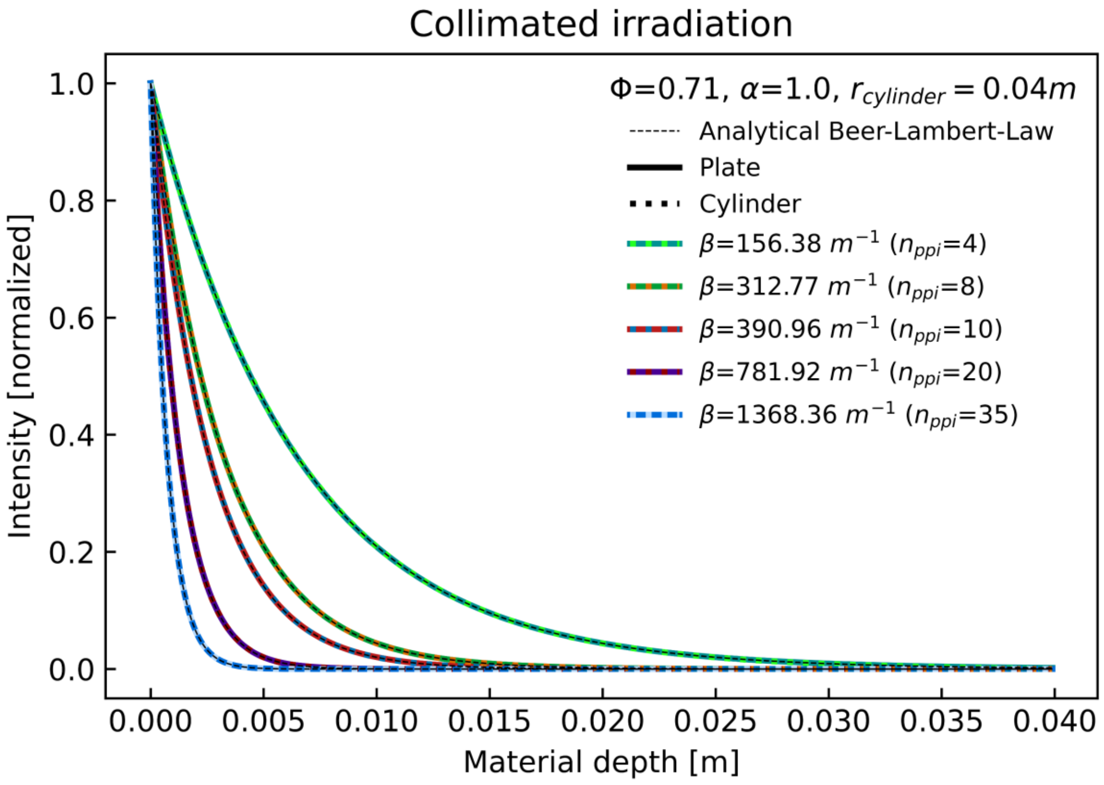
- Temperature swing operation requires reheating of reactor components after each cycle
- Direct irradiation of RPC structure from one site results in significant **temperature gradient along material thickness:**
  - Inhomogeneous reduction extent δ
  - Overheating of RPC front can cause higher reradiation losses and structural damage



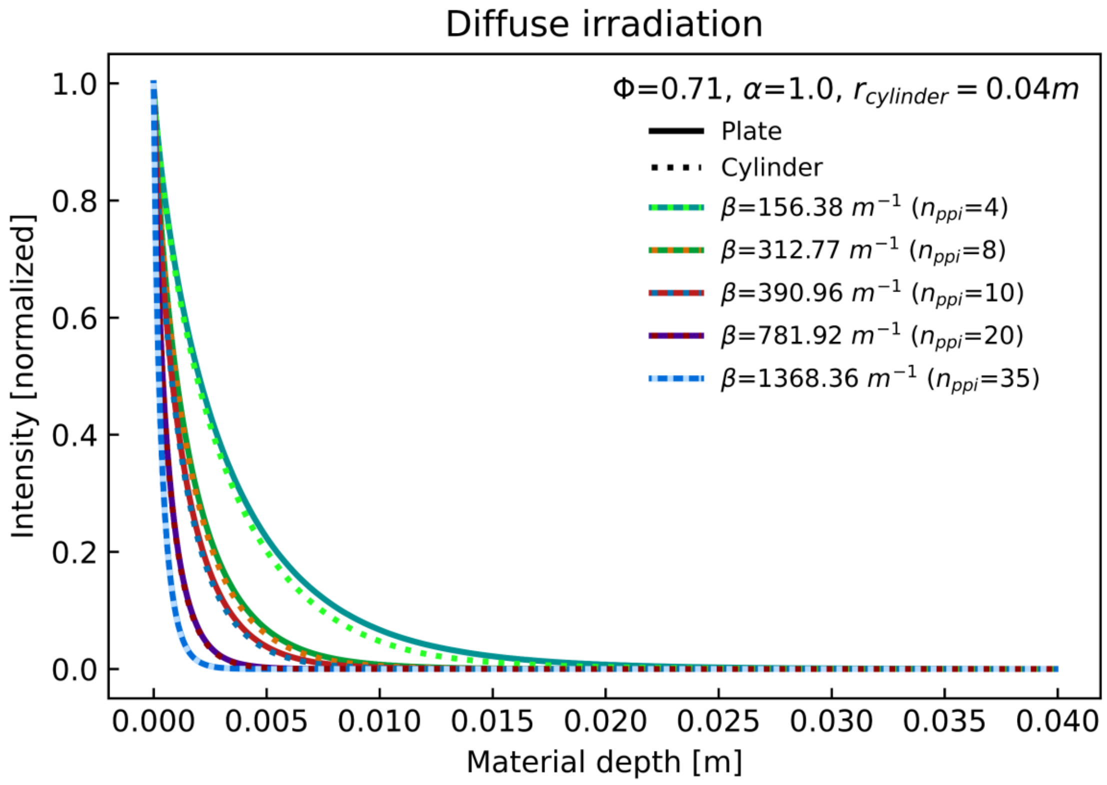
M. Hoes, S. Ackermann, D. Theiler, P. Furler, and A. Steinfeld, Energy Technol. 7, 1900484 (2019).

Modeling Results

Variation of Extinction Coefficient β (n_{ppi} variation)



Collimated irradiation

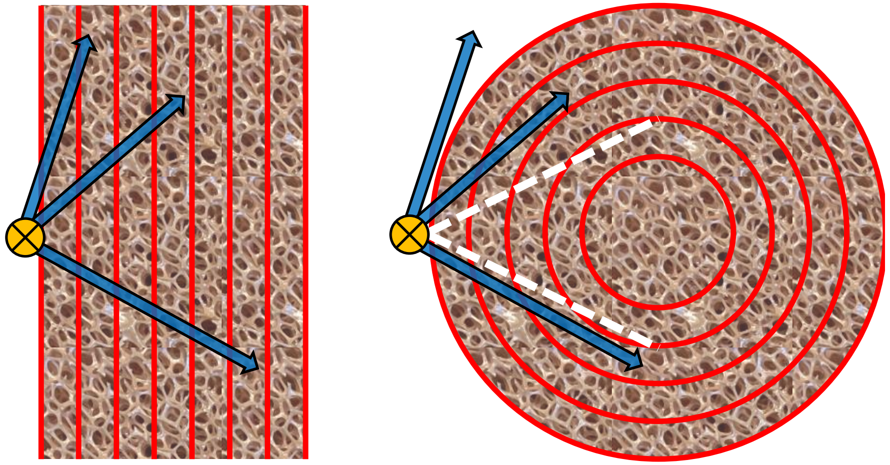


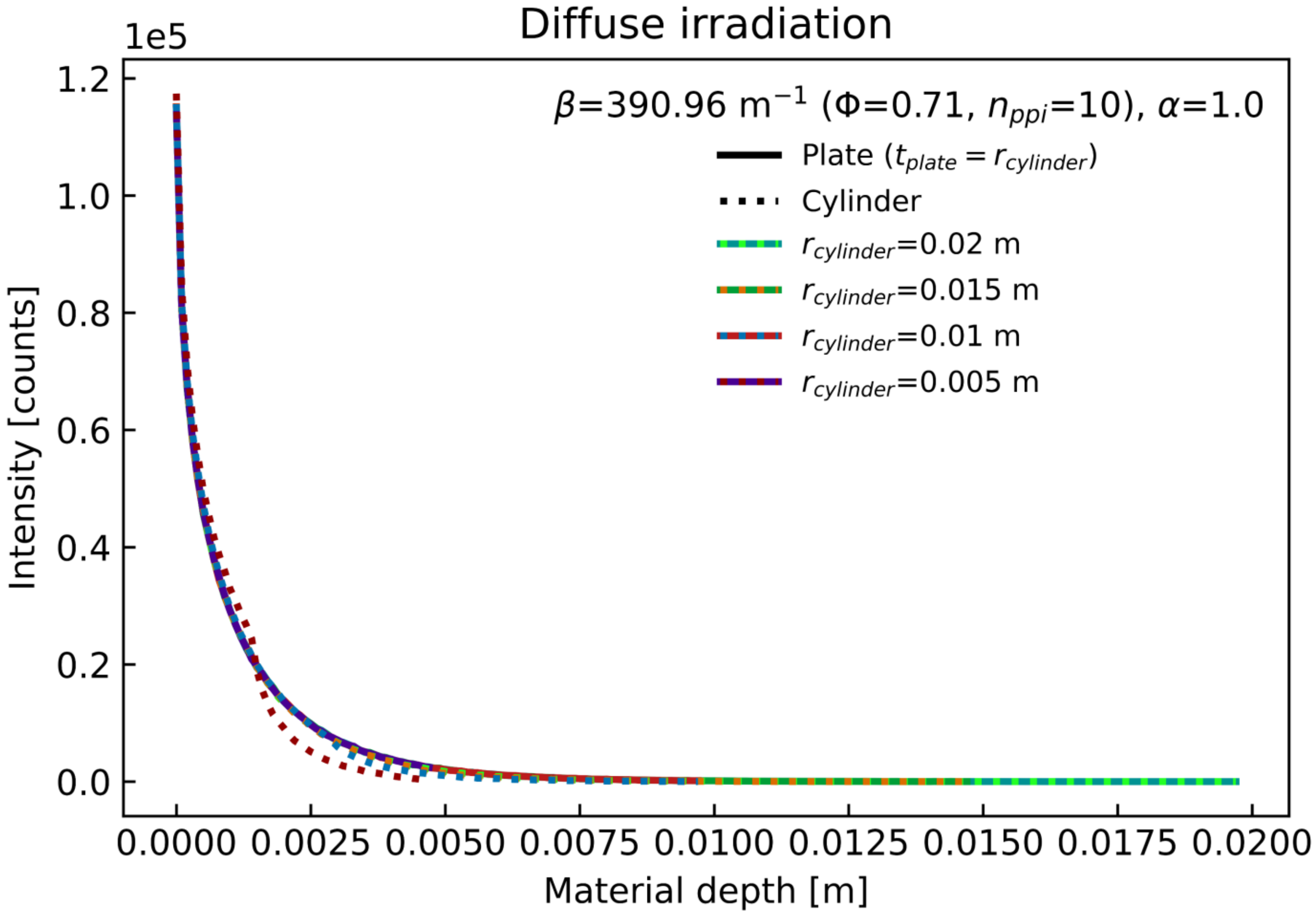
Diffuse irradiation

Modeling Results: Intensity attenuation

Variation of Cylinder Radius / Material Thickness

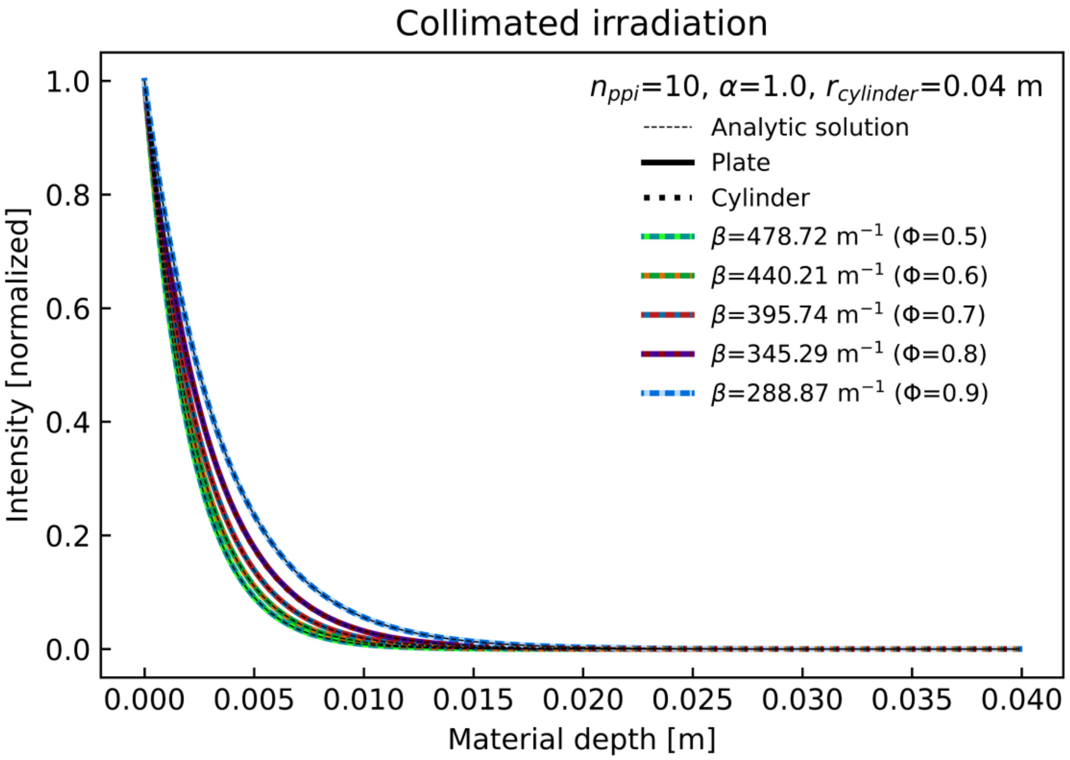
- For smaller cylinder radii the range of incident angles for rays reaching inner radial segments decreases
- For cylinder a larger fraction of total volume is located in outer segments compared to plate

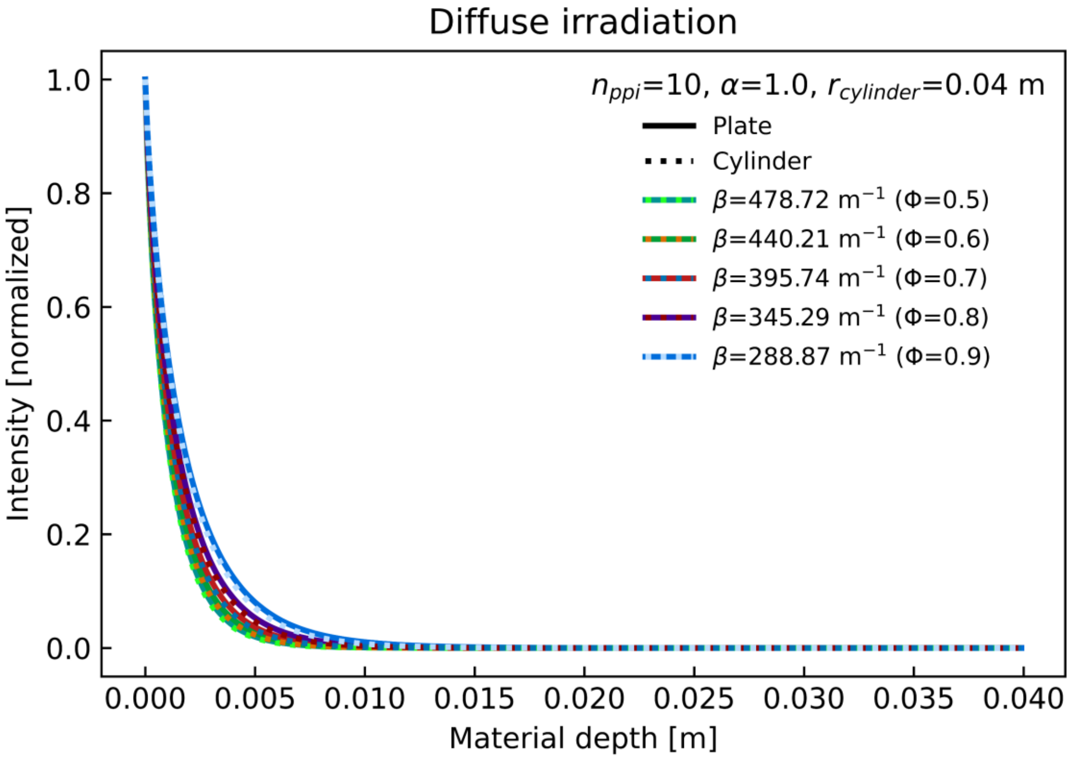




Modeling Results

Variation of Extinction Coefficient β (ϕ variation)

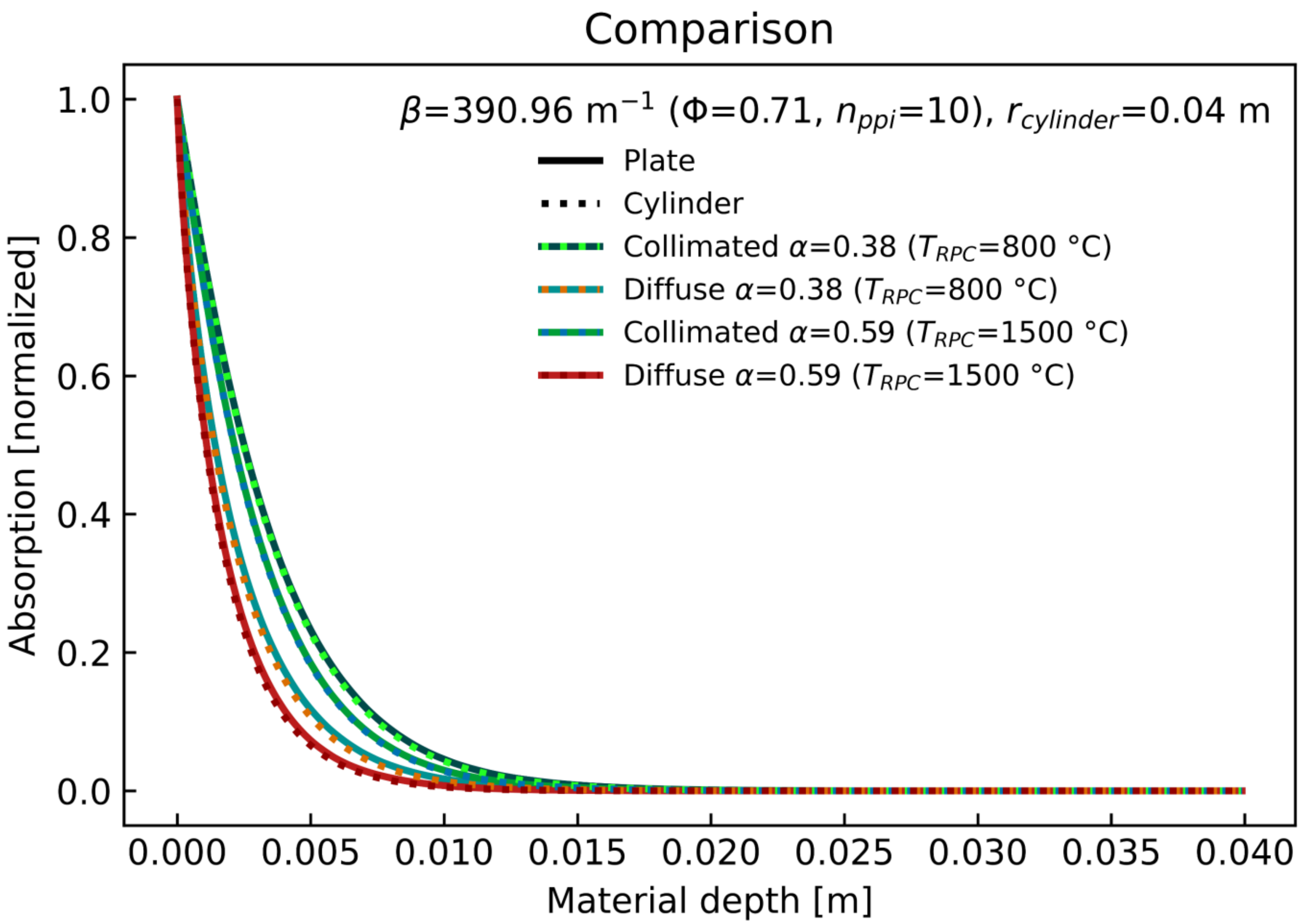




Modeling Results

Variation of Absorptivity α (δ variation)

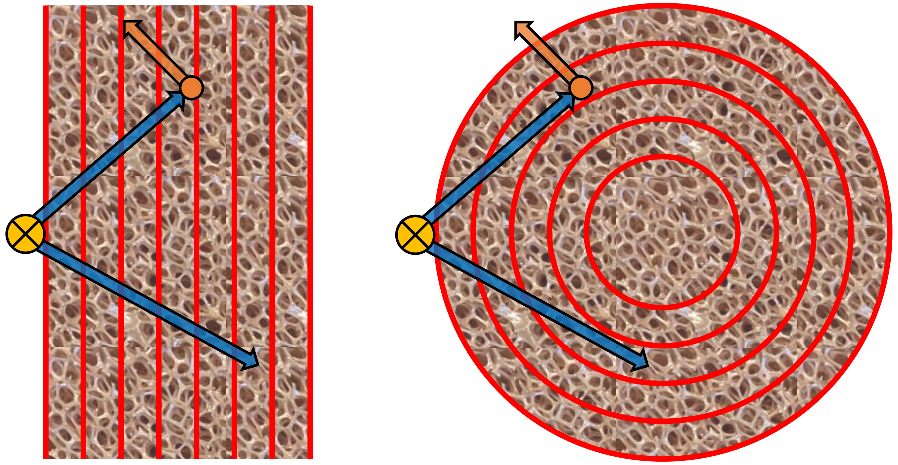
- For large cylinder absorption characteristics follows similar trend as intensity attenuation
- For smaller extinction coefficients radiation can scatter more easily out of RPC structure

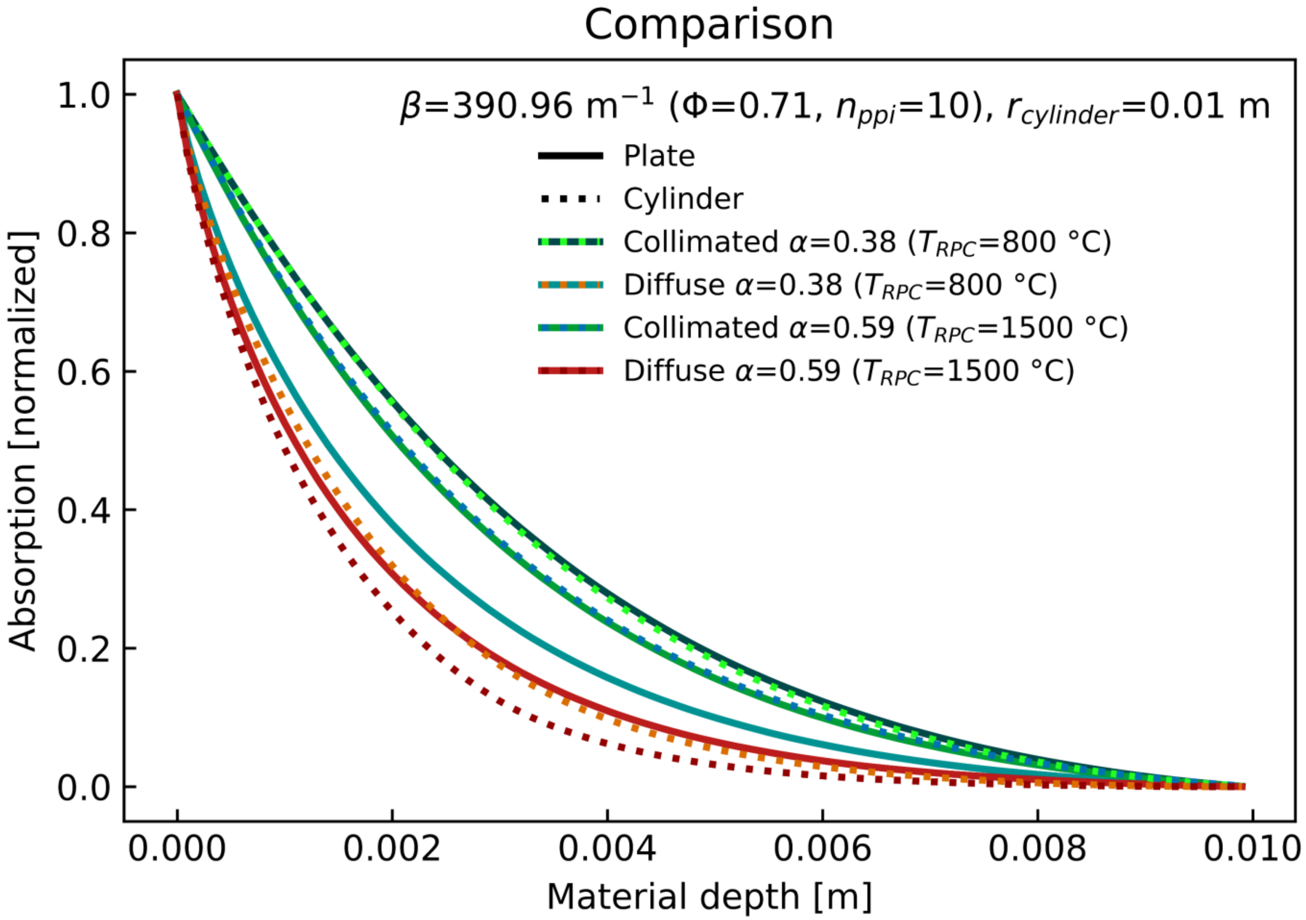


Modeling Results

Variation of Absorptivity α (δ variation) – Small Cylinder

- Rays scatter more easily out of small cylinder due to radial confinement, effect decreases with increasing absorptivity





Imprint

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