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Pressure Separation and Gas Flows in a Prototype Vacuum-Pumped Solar-Thermochemical Reactor

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Fuel Cell Technologies Office

Outline

- A
- B
- C

- D
- E
- F

Two-Step Thermochemical Fuel Production

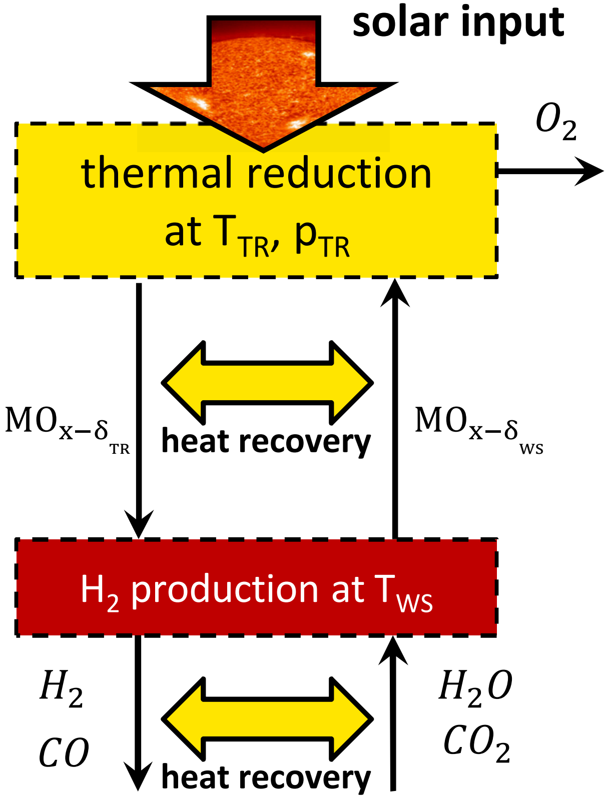
Thermal reduction

$$\frac{1}{\delta_{TR} - \delta_{WS}} MO_{x-\delta_{WS}} \rightarrow \frac{1}{\delta_{TR} - \delta_{WS}} MO_{x-\delta_{TR}} + \frac{1}{2} O_2$$

Water/CO_2 splitting

$$\frac{1}{\delta_{TR} - \delta_{WS}} MO_{x-\delta_{TR}} + H_2O \rightarrow \frac{1}{\delta_{TR} - \delta_{WS}} MO_{x-\delta_{WS}} + H_2$$

$$\frac{1}{\delta_{TR} - \delta_{WS}} MO_{x-\delta_{TR}} + CO_2 \rightarrow \frac{1}{\delta_{TR} - \delta_{WS}} MO_{x-\delta_{WS}} + CO$$



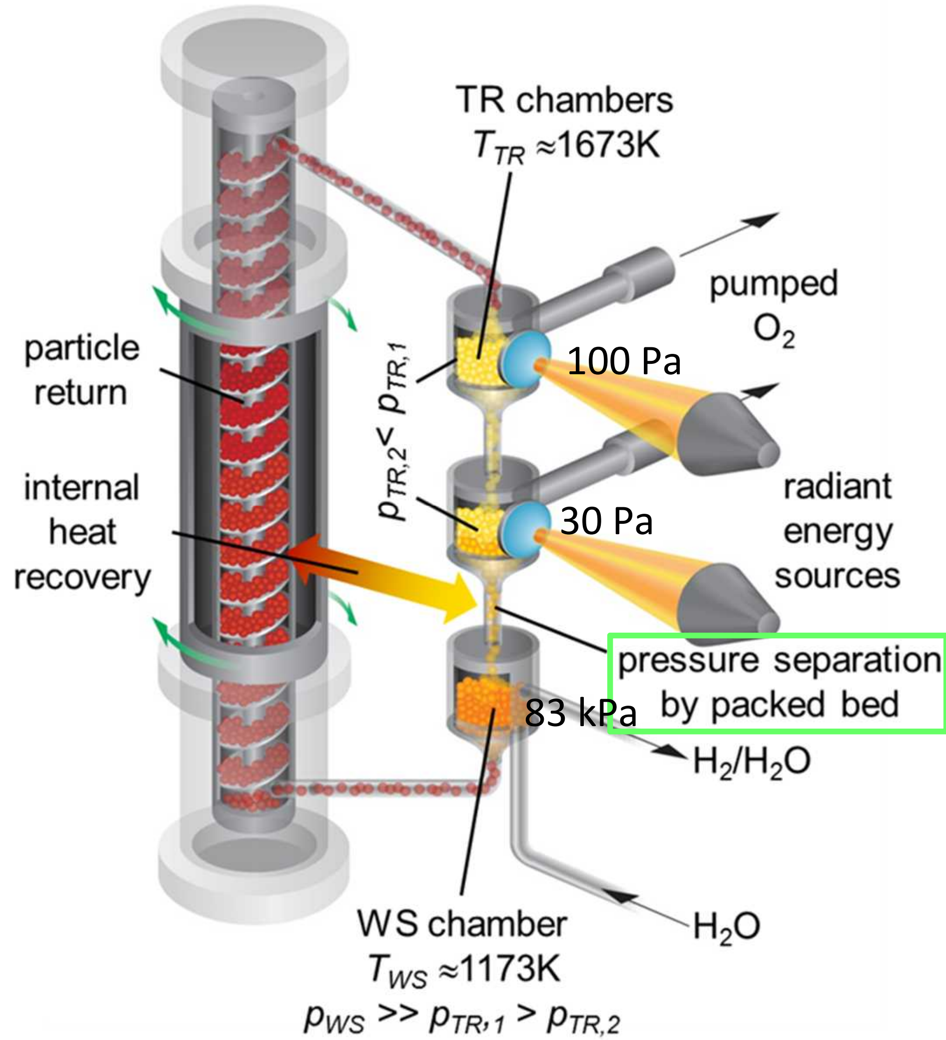
A theoretically simple process

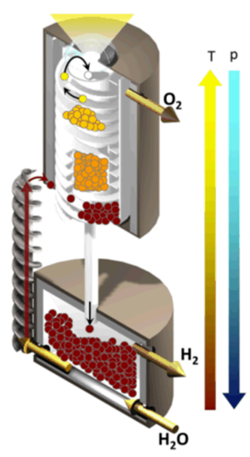
Cascading Pressure Reactor

An improvement of an earlier moving packed bed concept

- Direct solar absorption
- Internal heat recovery between T_{TR} and T_{WS}
- Continuous on-sun operation
- Temperature and product separation
- Pressure separation (thermal reduction step vacuum pumping)
- Non-monolithic oxide
- Reaction kinetics decoupled from reactor operation

- Thermal reduction pressure (0.1-10Pa)
- Decreased solid-solid heat recovery requirement
- Decreased pump work requirement
- Compatibility with MW-scale plant





Gas Permeation: The Simple Approach

Darcy flow for compressible fluids:

$$Q_{p_h - p_l, p_r} = \frac{KA(p_h^2 - p_l^2)}{2\mu L p_r} \qquad K = \frac{\varepsilon^{5.5} d^2}{5.6}$$

Goal 1: Minimize gas permeation between chambers.

Maximum pressure separation capacity:

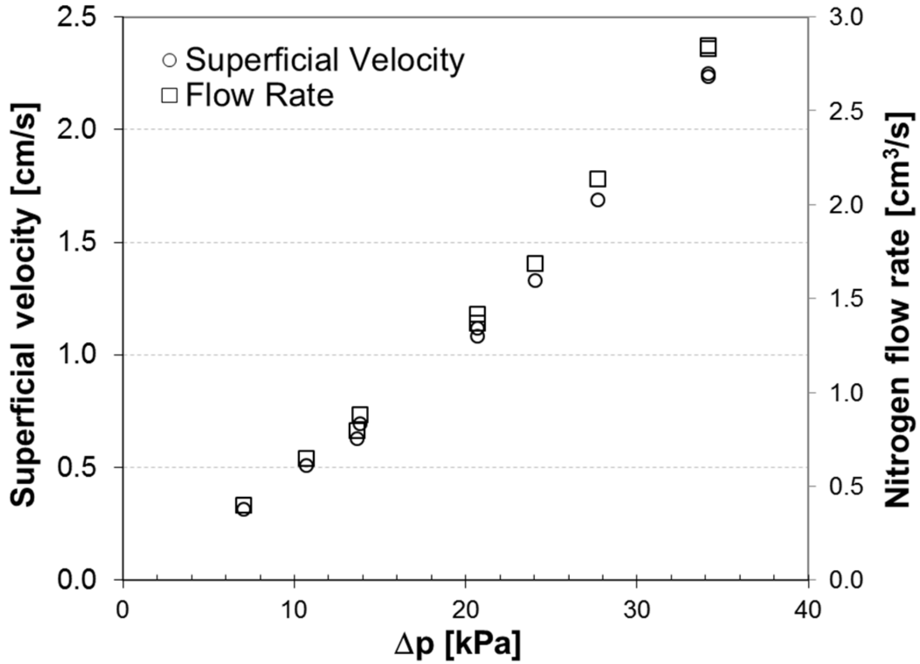
$\Delta p_{max} = \rho_{bulk} g h$

Fluidization at top: Stokes drag

$F_D = 6\pi\mu R v$

Goal 2: Keep connecting beds packed at all times.

Nitrogen flow rate through a 2.16m tall (ID=12.7mm) static column of steel grit (d~180μm)

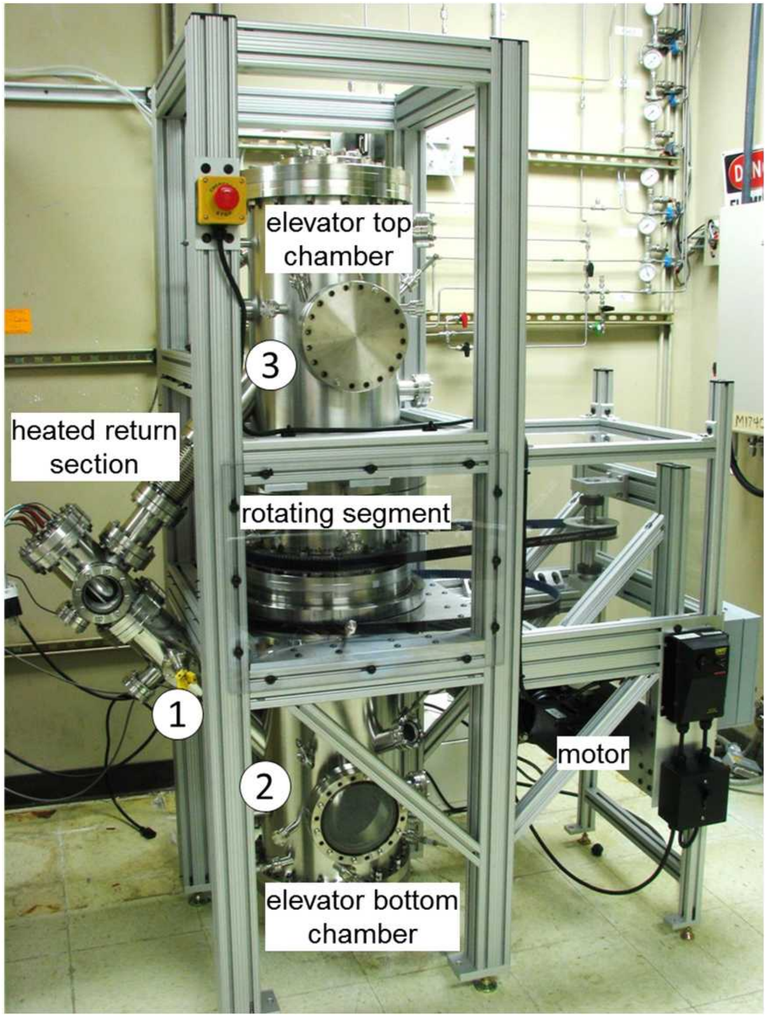


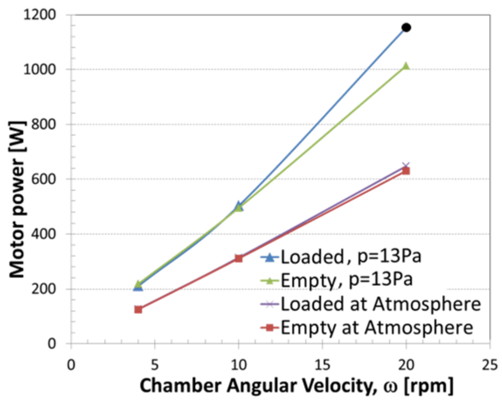
Onset of fluidization near top: Δp=79kPa

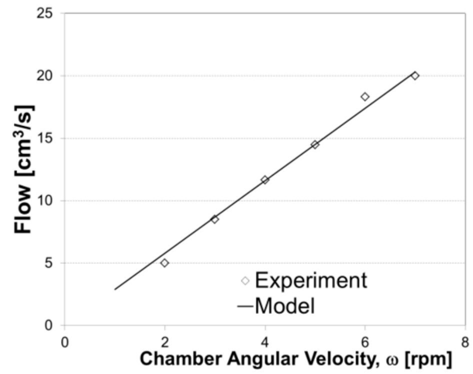
Predicted: Δp=76kPa

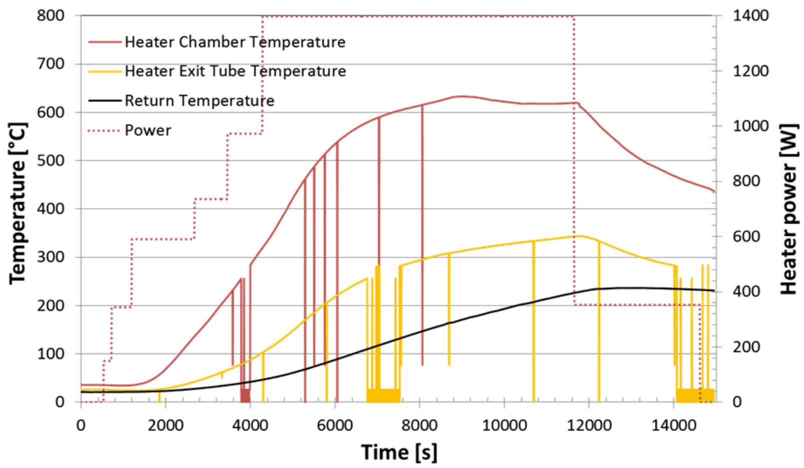
Pressure separation possible as predicted by model

Particle Elevation w/ Pressure Separation









- **Elevation – sufficient capacity**
- **Power requirement – comparatively small**
- **Pressure separation – demonstrated**

Gas Permeation: Detailed Approach

$$\frac{\mathrm{d}p}{\mathrm{d}\boldsymbol{l}} = -\frac{\dot{m}_g}{A(l)}\frac{RT}{pMD_p}\frac{1-\phi}{\phi^3}\left[\frac{150(1-\phi)\mu}{f_c\,(Kn)D_p} + 1.75\frac{\dot{m}_g}{A(l)}\right]$$

Ergun equation with Knudsen correction

$$f_c = [1+\alpha(Kn)Kn]\left[1+\frac{4Kn}{1-bKn}\right]$$

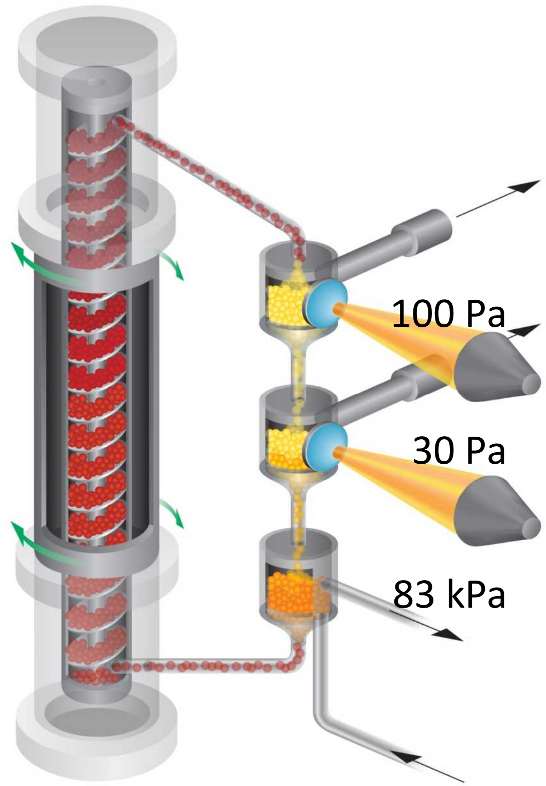
Knudsen correction factor

$$Kn = \frac{\lambda}{D_p} \qquad \lambda = \frac{k_B T}{\sqrt{2}\pi d^2 p}$$

$$\alpha(Kn) = \alpha_0 \frac{2}{\pi} tan^{-1}\left(\alpha_1 Kn^{\beta}\right)$$

$$\alpha_0 \equiv \alpha_{Kn\to\infty} = \frac{64}{3\pi\left(1-\frac{4}{b}\right)}$$

Must use full equations because of substantial pressure drops

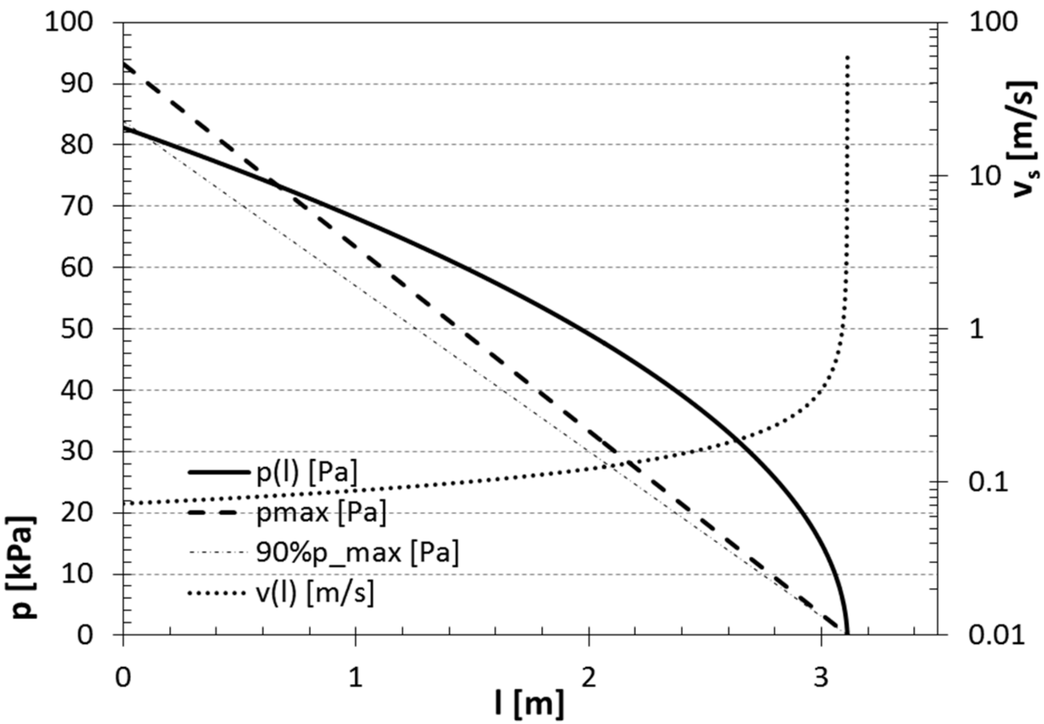


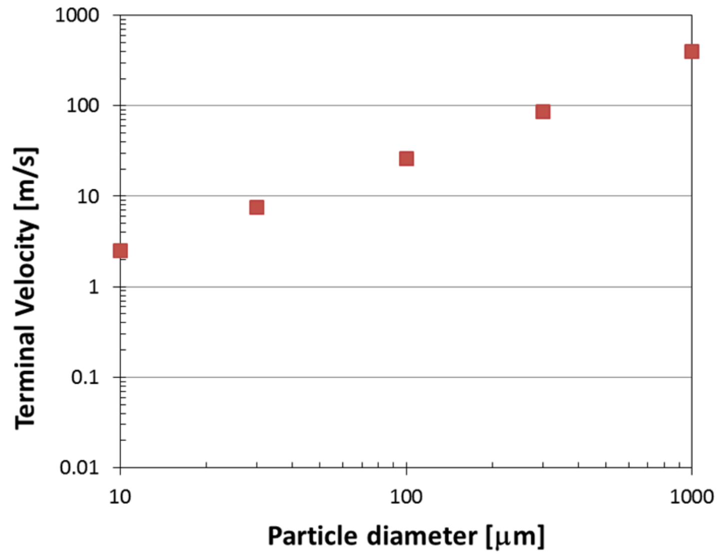
First Obstacle: Gas Expansion

$$\frac{\mathrm{d}p}{\mathrm{d}\boldsymbol{l}} = -\frac{\dot{m}_g}{A(l)}\frac{RT}{pMD_p}\frac{1-\phi}{\phi^3}\left[\frac{150(1-\phi)\mu}{f_c\,(Kn)D_p} + 1.75\frac{\dot{m}_g}{A(l)}\right]$$

83 kPa→100 Pa H_2
T=800°C
ϕ=0.4
D_p=300 μm

ID=15 mm
incline=45°





Design must include flow diameter increases

Flow Expansion: Problem Solved?

$$\frac{\mathrm{d}p}{\mathrm{d}\boldsymbol{l}} = -\frac{\dot{m}_g}{A(l)}\frac{RT}{pMD_p}\frac{1-\phi}{\phi^3}\left[\frac{150(1-\phi)\mu}{f_c\,(Kn)D_p} + 1.75\frac{\dot{m}_g}{A(l)}\right]$$

83 kPa → 100 Pa H_2
T=800°C
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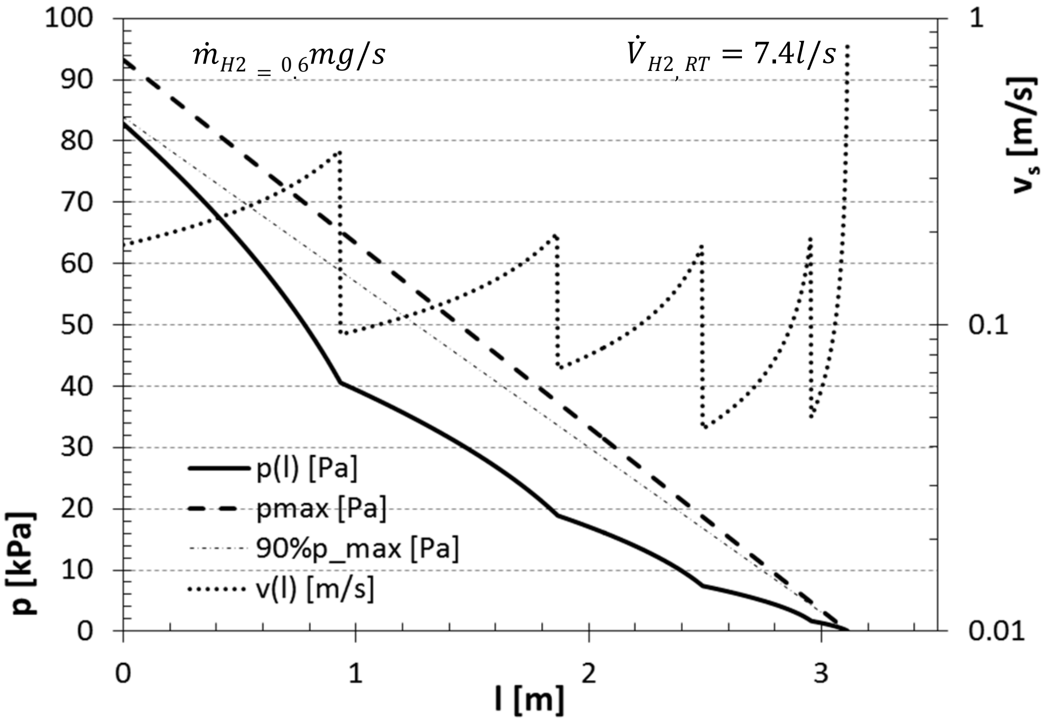
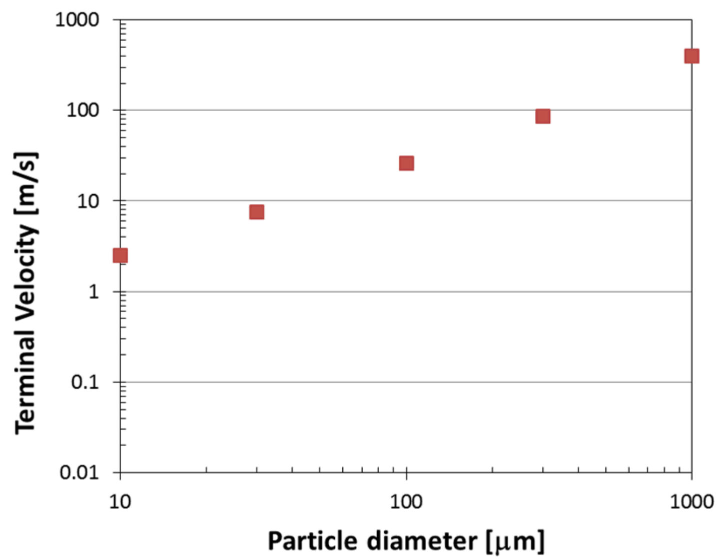
D_p=300 μm

ID_i=15 mm
ID_f=200 mm
incline=45°





But...

Second Obstacle: H_2-O_2 Recombination Loss

$$\frac{dp}{d\boldsymbol{l}} = -\frac{\dot{m}_g}{A(l)}\frac{RT}{pMD_p}\frac{1-\phi}{\phi^3}\left[\frac{150(1-\phi)\mu}{f_c\,(Kn)D_p} + 1.75\frac{\dot{m}_g}{A(l)}\right]$$

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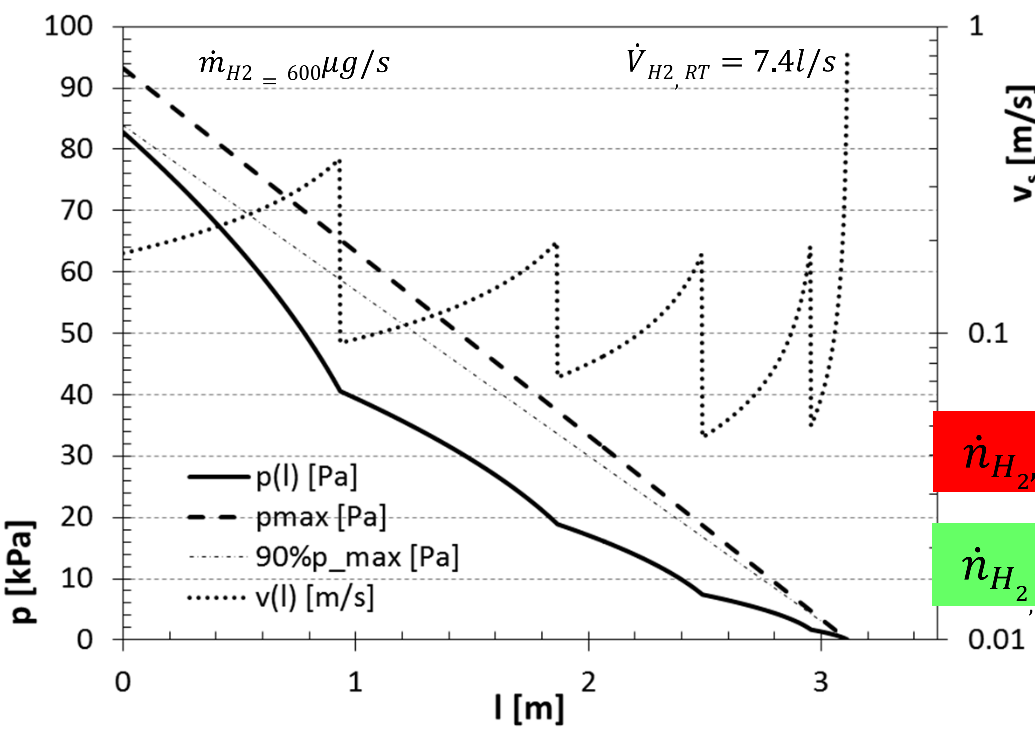
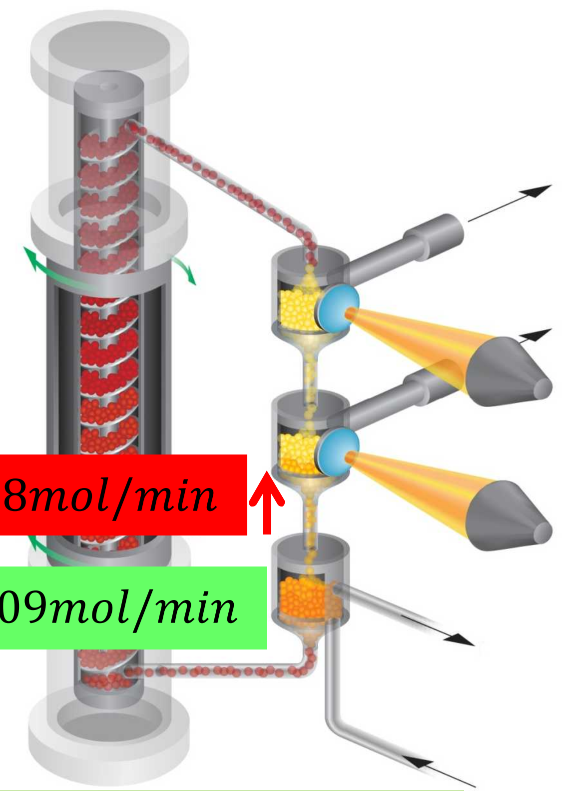




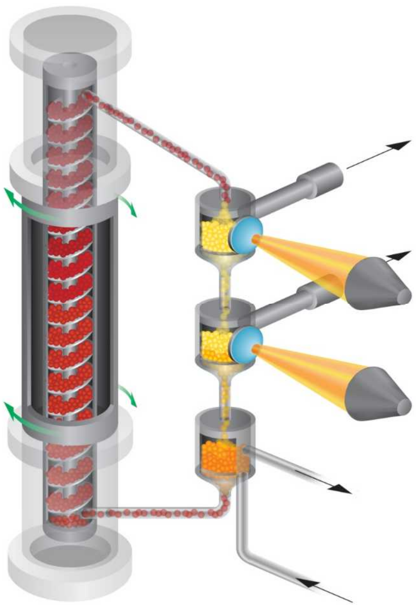
$\dot{n}_{H_2,loss} = 0.018 mol/min$

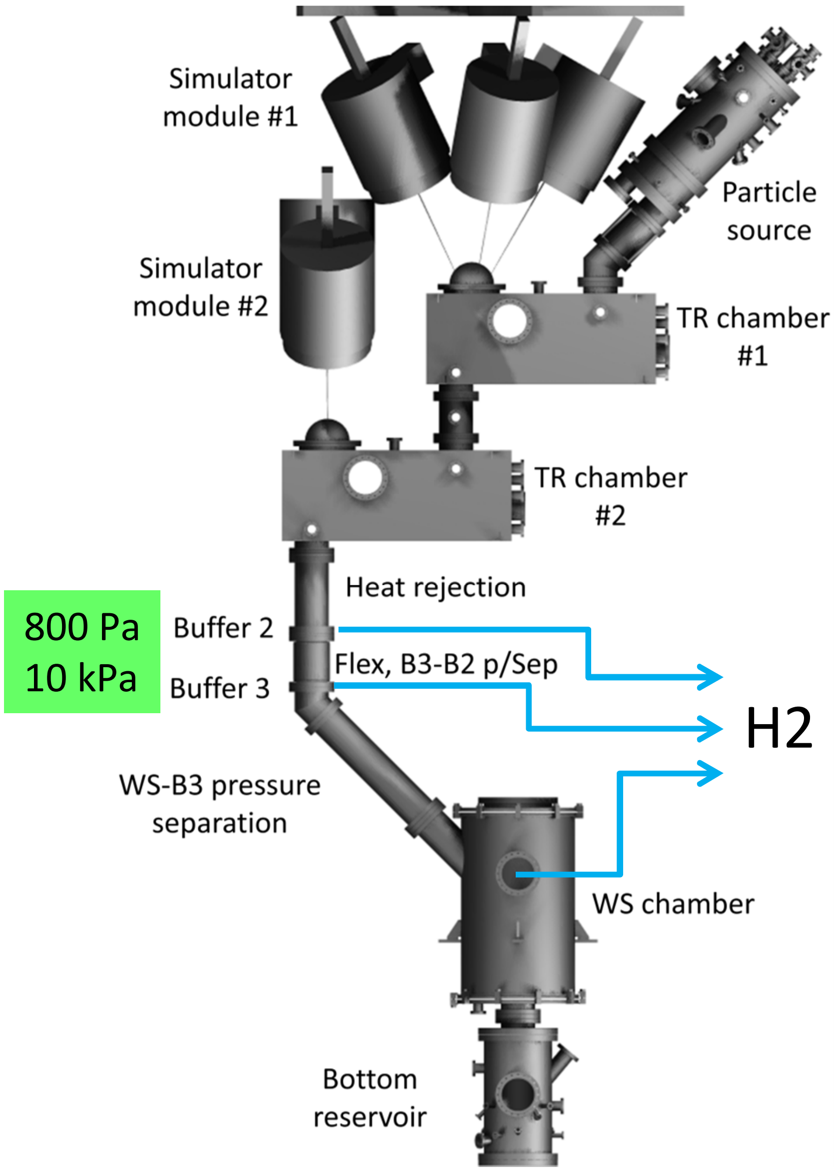
$\dot{n}_{H_2 prod.} = 0.009 mol/min$

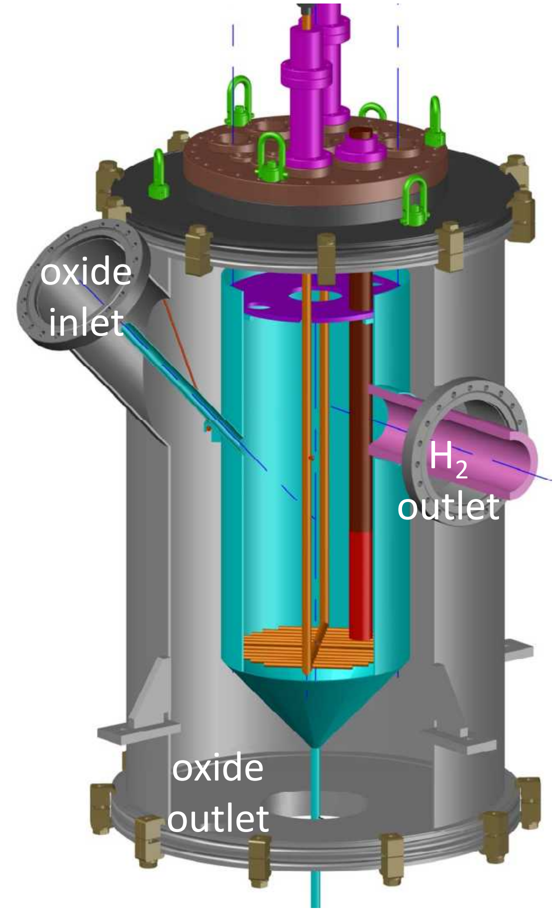
Staged flow expansion ensures pressure separation without fluidization

Gas flow to TR chamber must be significantly decreased

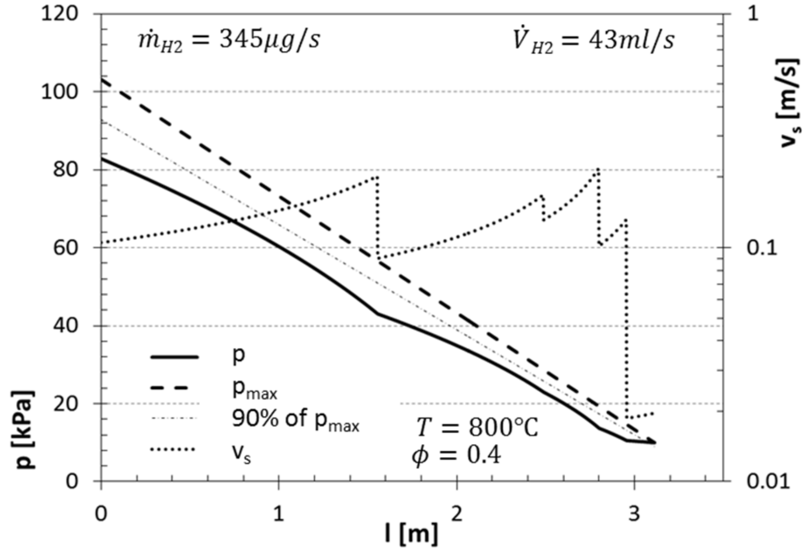
Putting it all Together





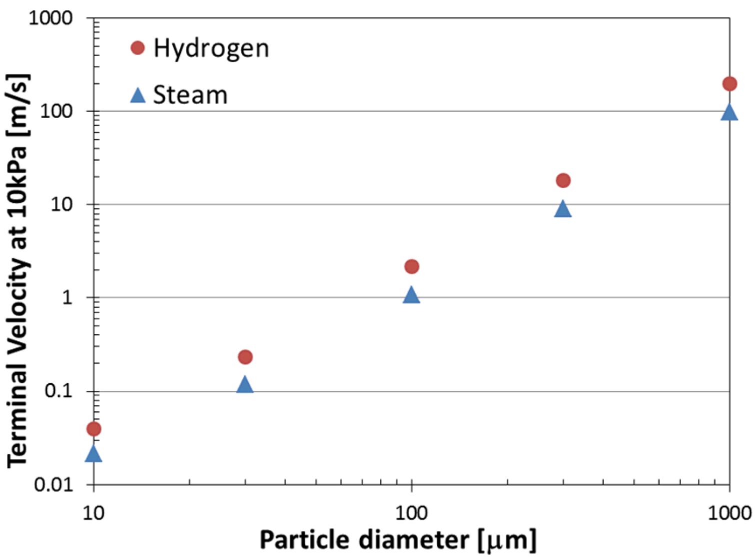


WS to Buffer 3 Permeation



83 kPa→10 kPa H_2
T=800°C
ϕ=0.4
D_p=300 μm

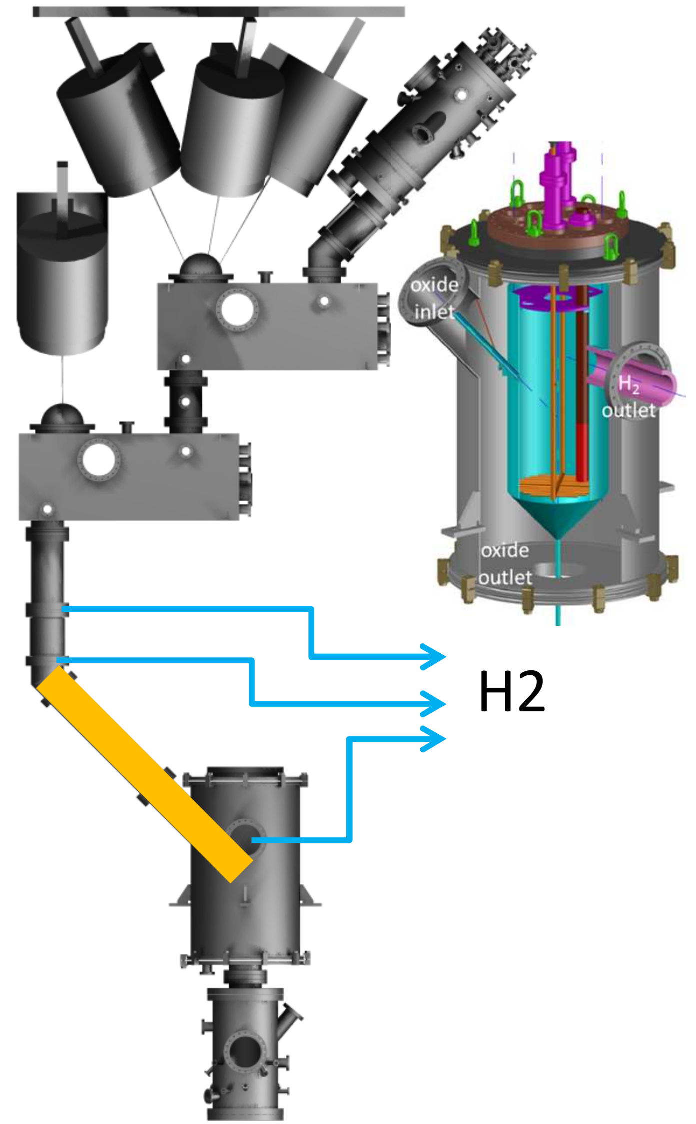
ID_i=15 mm
ID_f=50 mm
incline=45°



$$v_t = \frac{C(\rho_{solid} - \rho_{gas})D_p}{18}$$

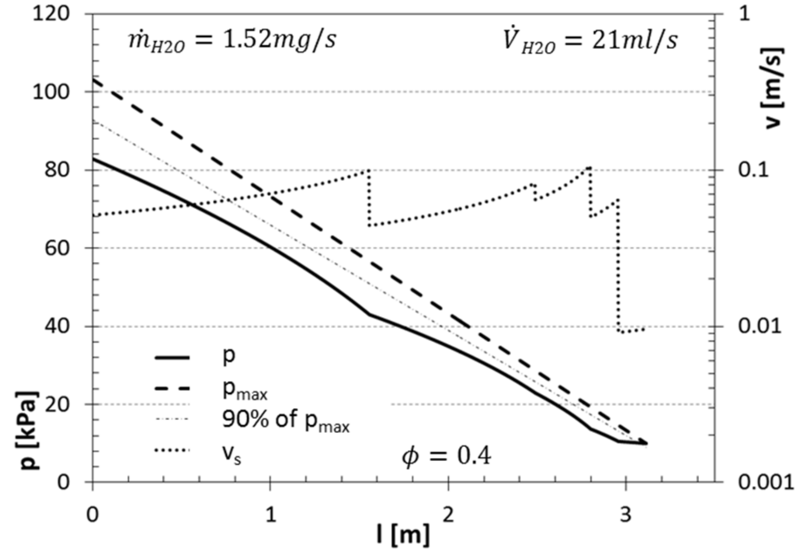
$$C = 1 + A \cdot Kn$$

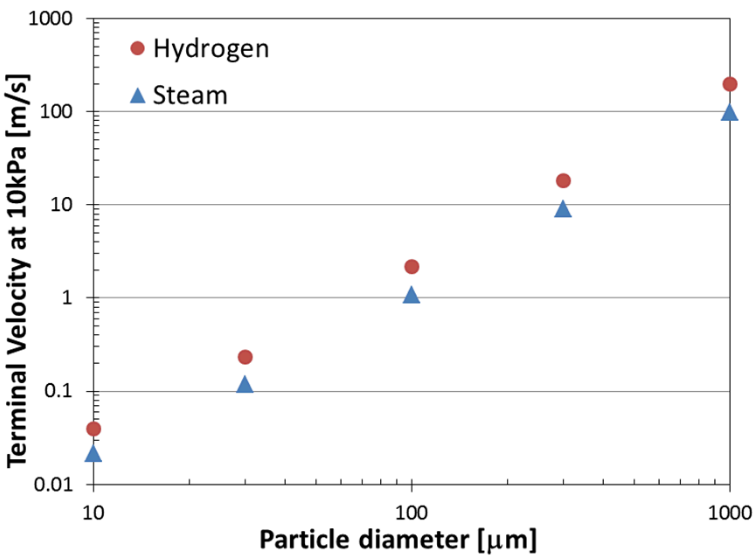
$$A = \alpha + \beta e^{\frac{-\gamma}{Kn}}$$



H_2 permeation volumetric flow vastly decreased

Permeation vs. Gas Species





83 kPa→10 kPa H_2O
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$$v_t = \frac{C(\rho_{solid} - \rho_{gas})D_p}{18}$$

$$C = 1 + A \cdot Kn$$

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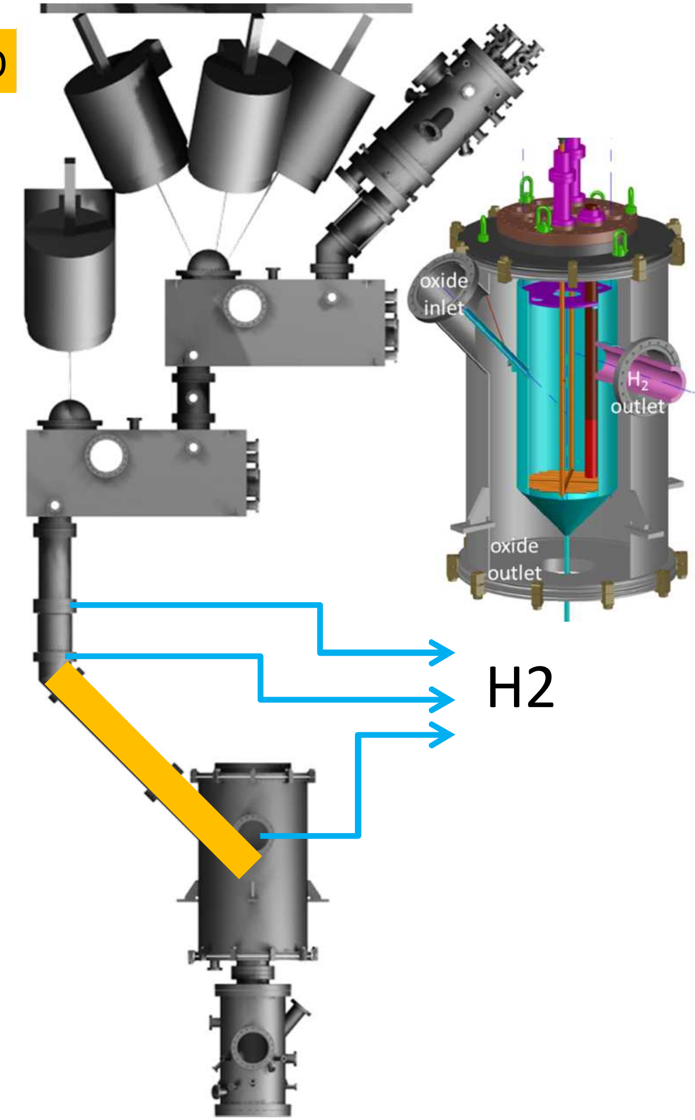
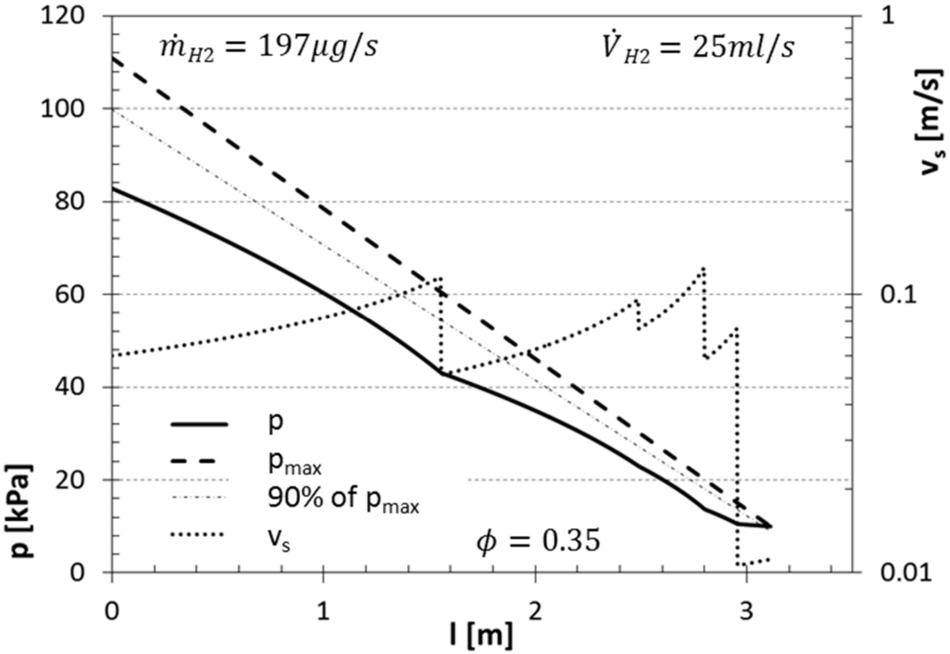
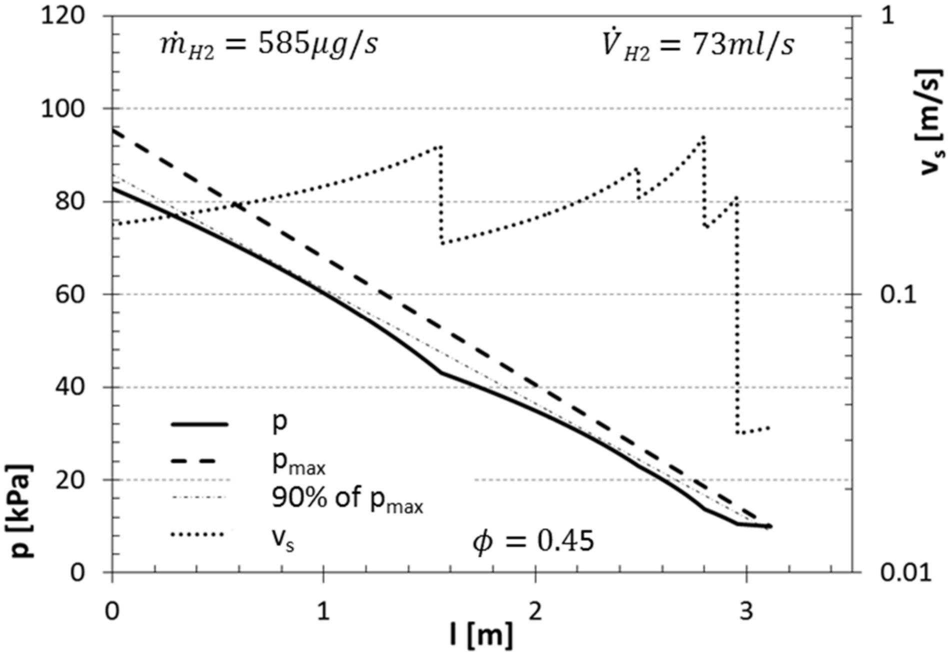


H_2 and H_2O pressure profiles are virtually identical

Permeation vs. Void Fraction



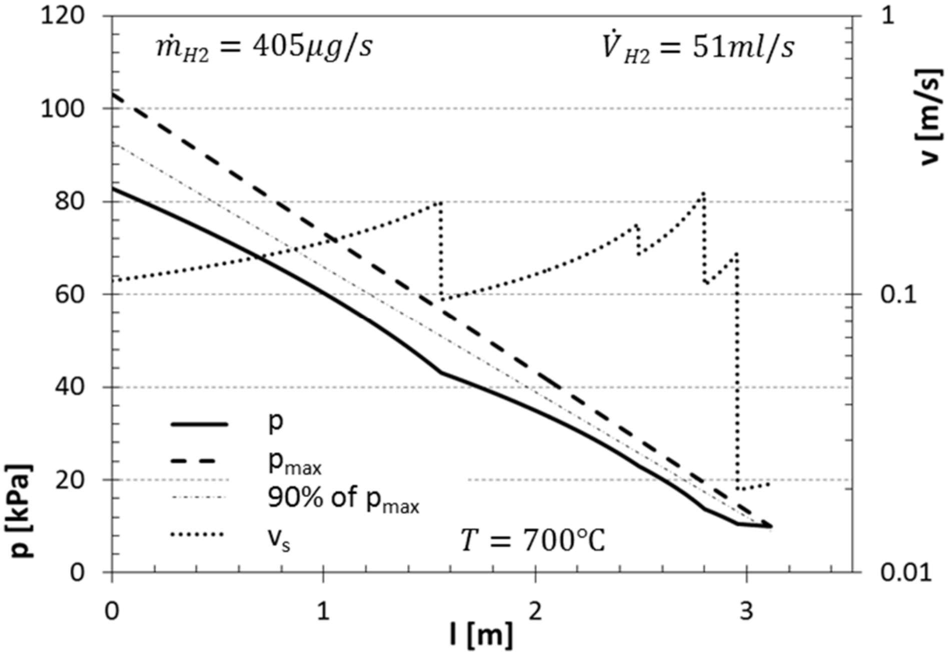
φ=0.35



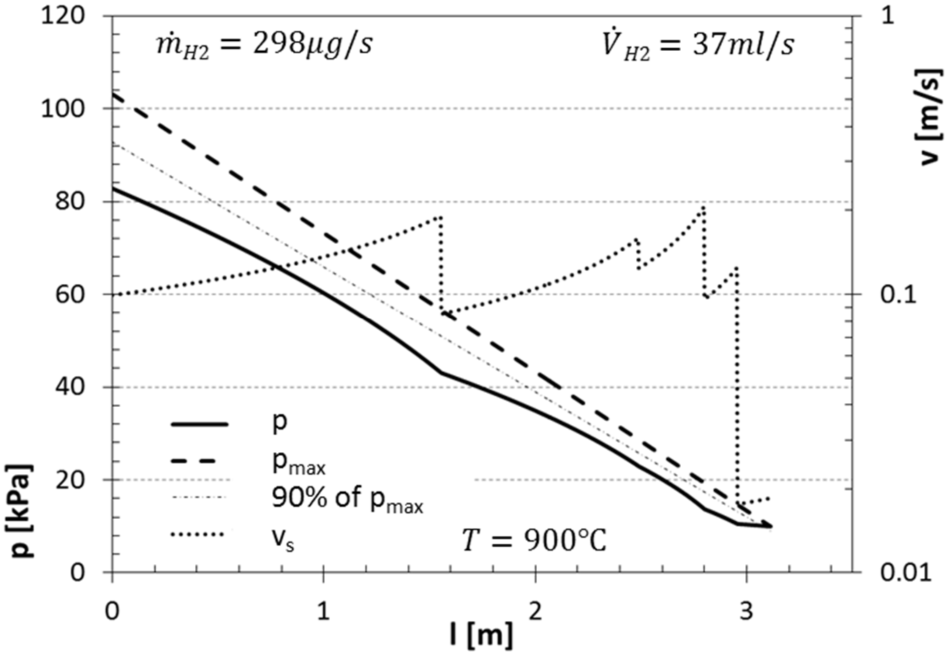
φ=0.45

Void fraction affects pressure separation capacity. Adequate margins are required.

Permeation vs. Temperature



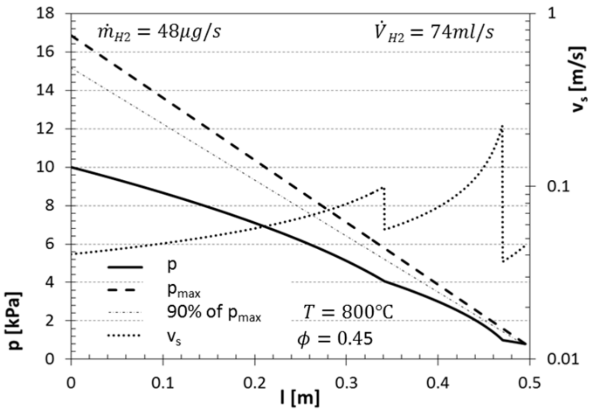
T=700°C

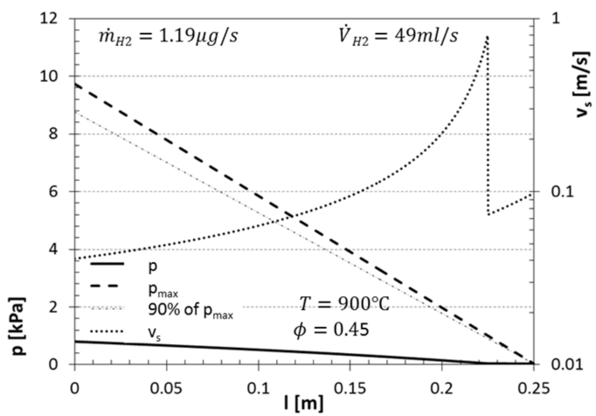


T=900°C

Temperature variations are of negligible importance

Buffer 3 to TR Chamber Permeation





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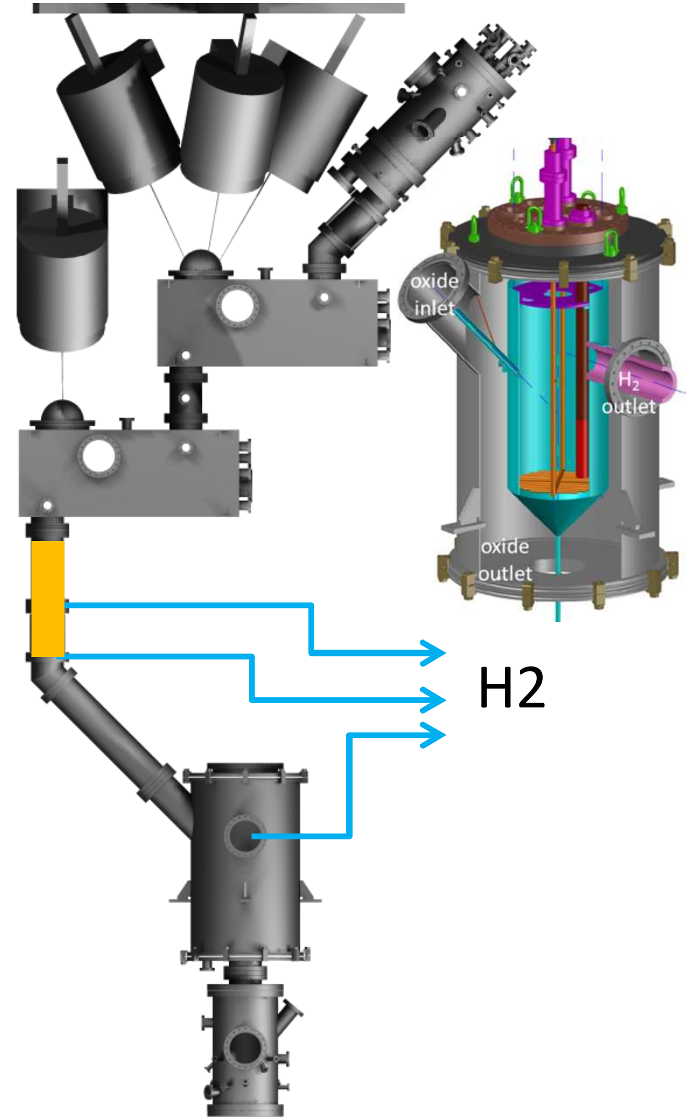
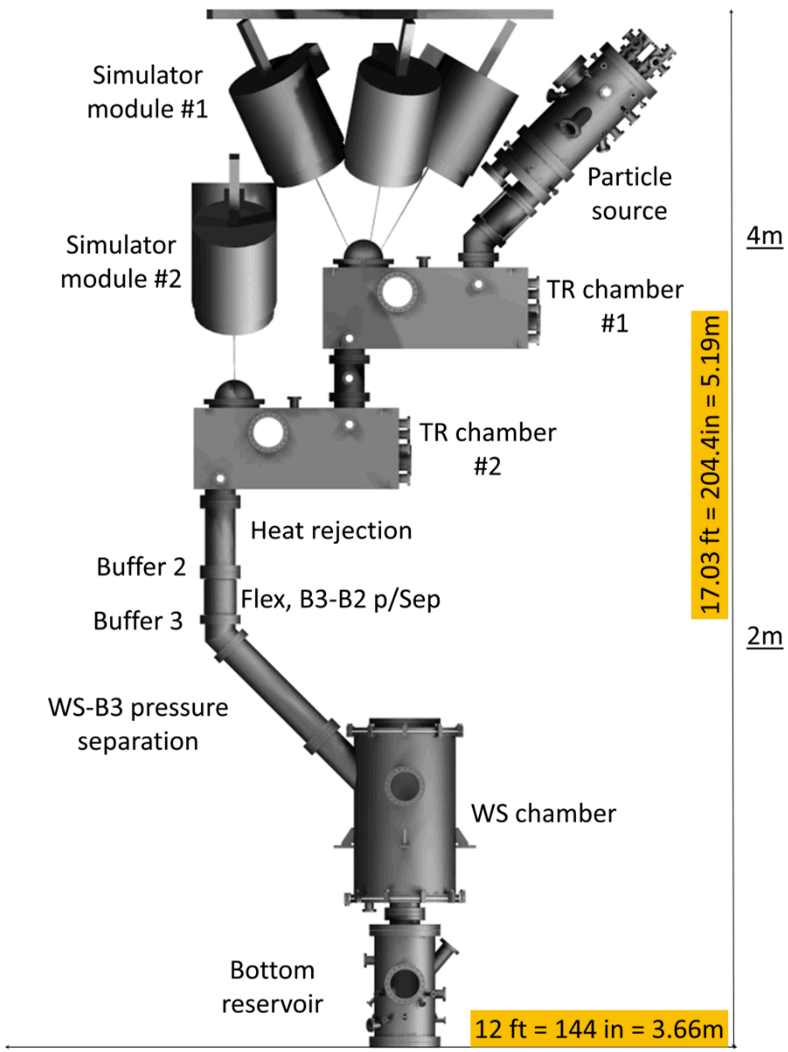


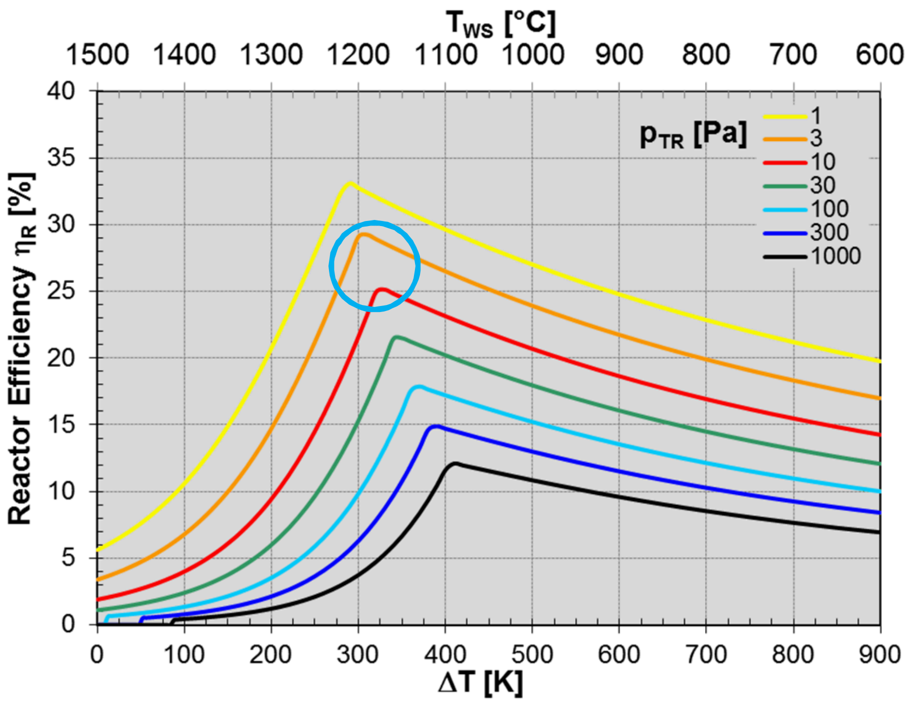
H_2 permeation volumetric flow vastly decreased

From Concept to Machine



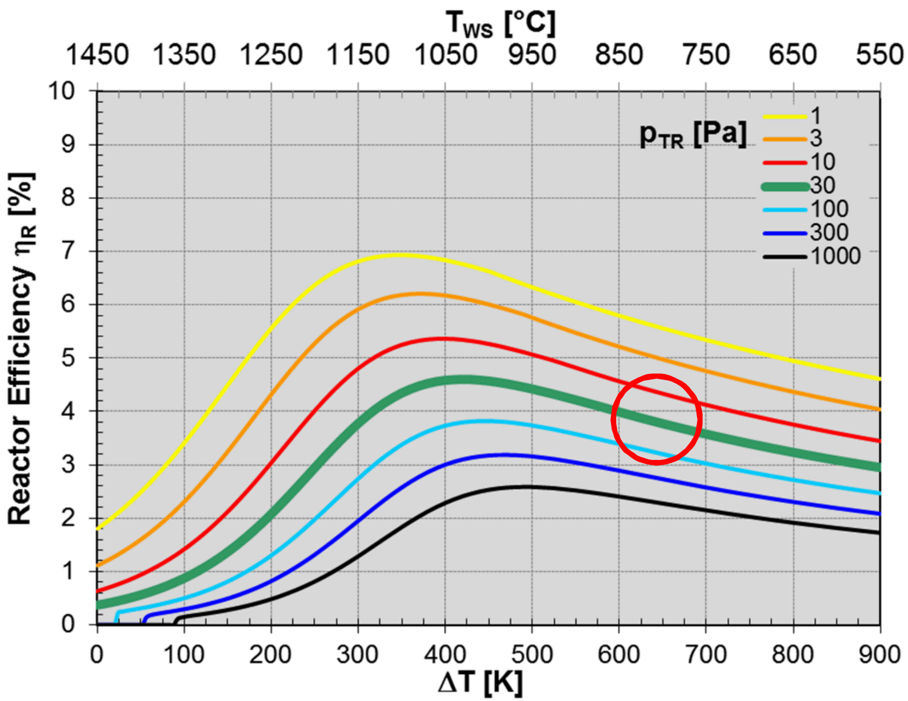
Reactor Efficiency: Two Limiting Cases

Ultimate CeO_2 Case



- T_{TR}=1500°C
- C=3000
- Extensive heat recovery
- Efficient pumping

First Prototype Target



- T_{TR}=1450°C
- C=1750
- No heat recovery
- Off-the-shelf pumps

- Existing components substantially affect efficiency
- Low reduction pressure of great importance

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Summary

- **Thermal reduction pressure limited by O_2 flow**
- **>10x pressure decrease feasible in staged reduction**
- **Pressure separation modeled and tested**
- **Particle elevation at high T, in vacuum, with pressure separation demonstrated**
- **Stick-slip receiver design**
- **Countercurrent flow WS chamber design**

Thank you

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