



X_{tended} **D**_{iscrete} **E**_{lement} **M**_{ethod}

Research Team

3D Modellierung von Festbettreaktoren mit Hilfe der XDEM

RUES

RESEARCH UNIT
IN ENGINEERING
SCIENCES



UNIVERSITÉ DU
LUXEMBOURG

Inhalt

- **Motivation**
 - Thermochemische Reaktoren
- **eXtended Discrete Element Method (XDEM)**
- **Multiphasen Modellierung**
 - Einzelpartikel
 - Granulares Medium/Festbett
- **Zusammenfassung und Ausblick**

Thermochemische Reaktoren I

Hochofen

Sinterbett

Koksofen



Thermochemische Reaktoren II

Wirbelschichtreaktoren



Vorschubrost

Hochofenprozess

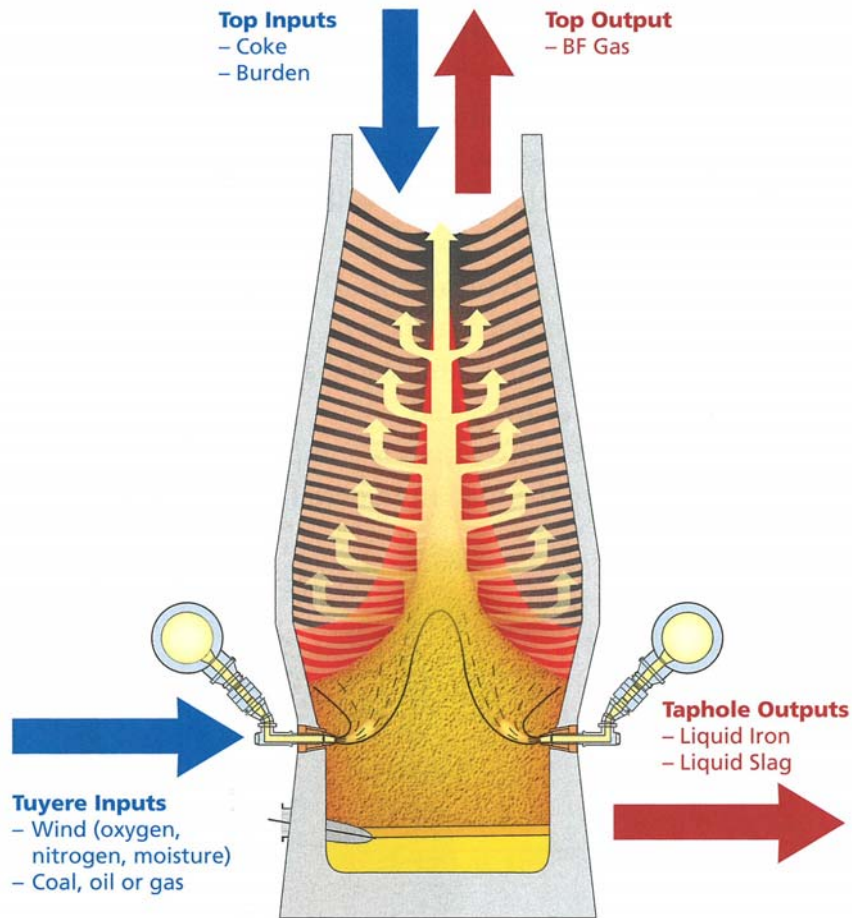


Image source: "Modern Blast Furnace Ironmaking – An introduction", M. Geerdes et al.

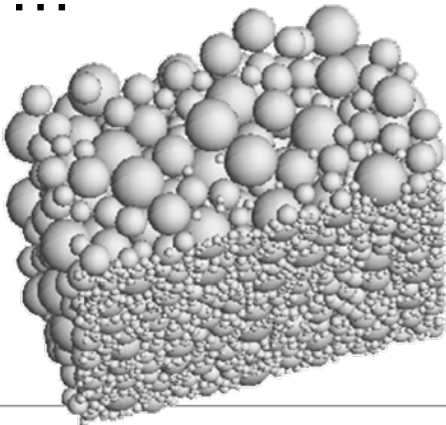
- “Ungemütliche” Prozessumgebung (300-1400° C, staubig, CO/CO₂)
- Multiphasensystem
 - Fest (Koks, Sinter, Pellets, Staub, ...)
 - Gas
 - Flüssig (Roheisen, Schlacke(n))
- Prozesse
 - Chemische Reaktion
 - Wärmetransport
 - Stofftransport
 - Fluidströmungen
 - Festkörperbewegung

eXtended Discrete Element Method (XDEM)

Simulationswerkzeug zur Modellierung granularer Medien und thermochem. Prozesse

Partikel Bewegung

- Sand
- Schnee
- ...

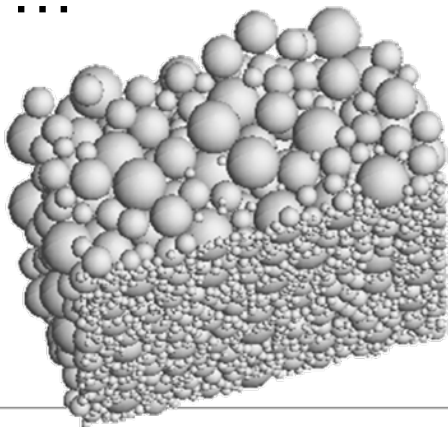


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Simulationswerkzeug zur Modellierung granularer Medien und thermochem. Prozesse

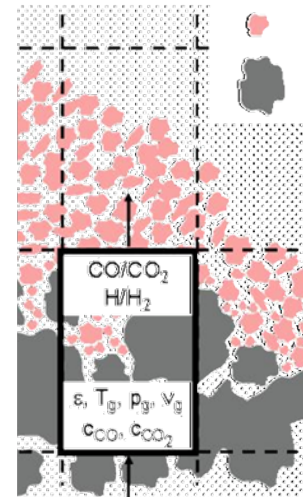
Partikel Bewegung

- Sand
- Schnee
- ...



Chemische Prozesse

- Trocknung
 - Verbrennung
 - Vergasung
 - Reduktion
- Koks, Pellets, Sinter,
Biomasse, Müll, ...

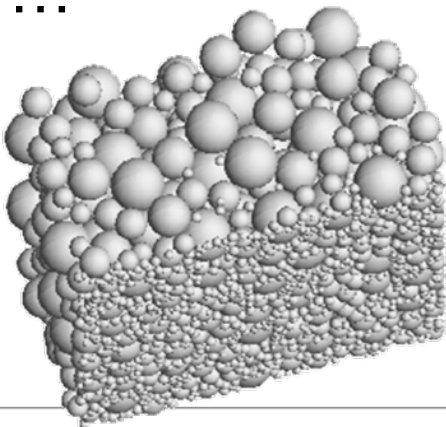


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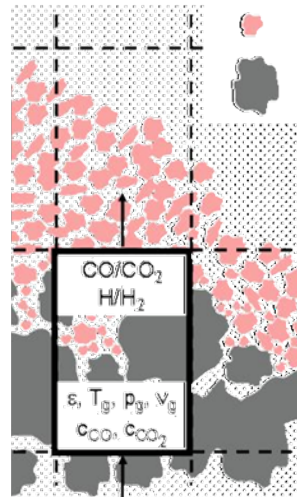


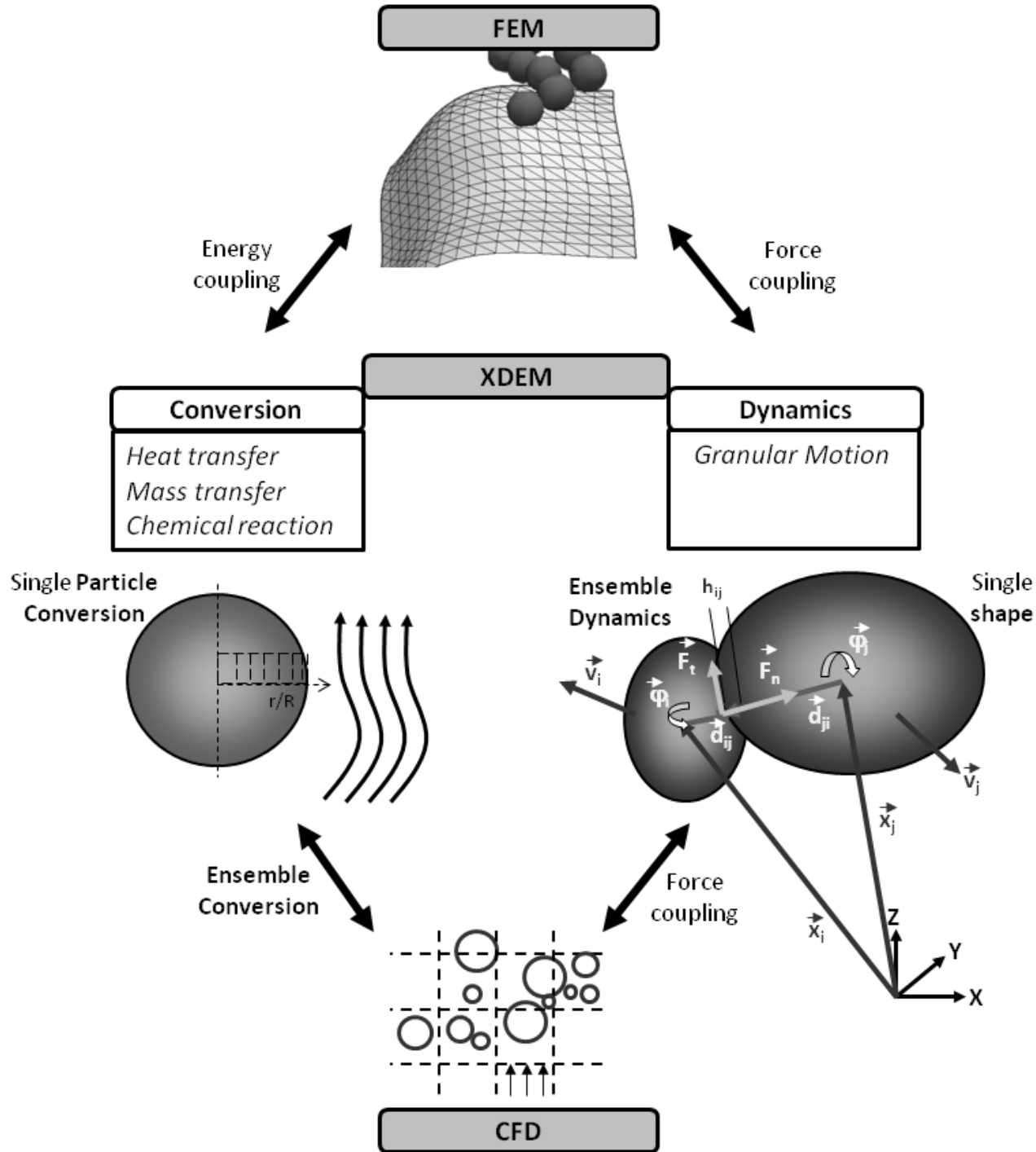
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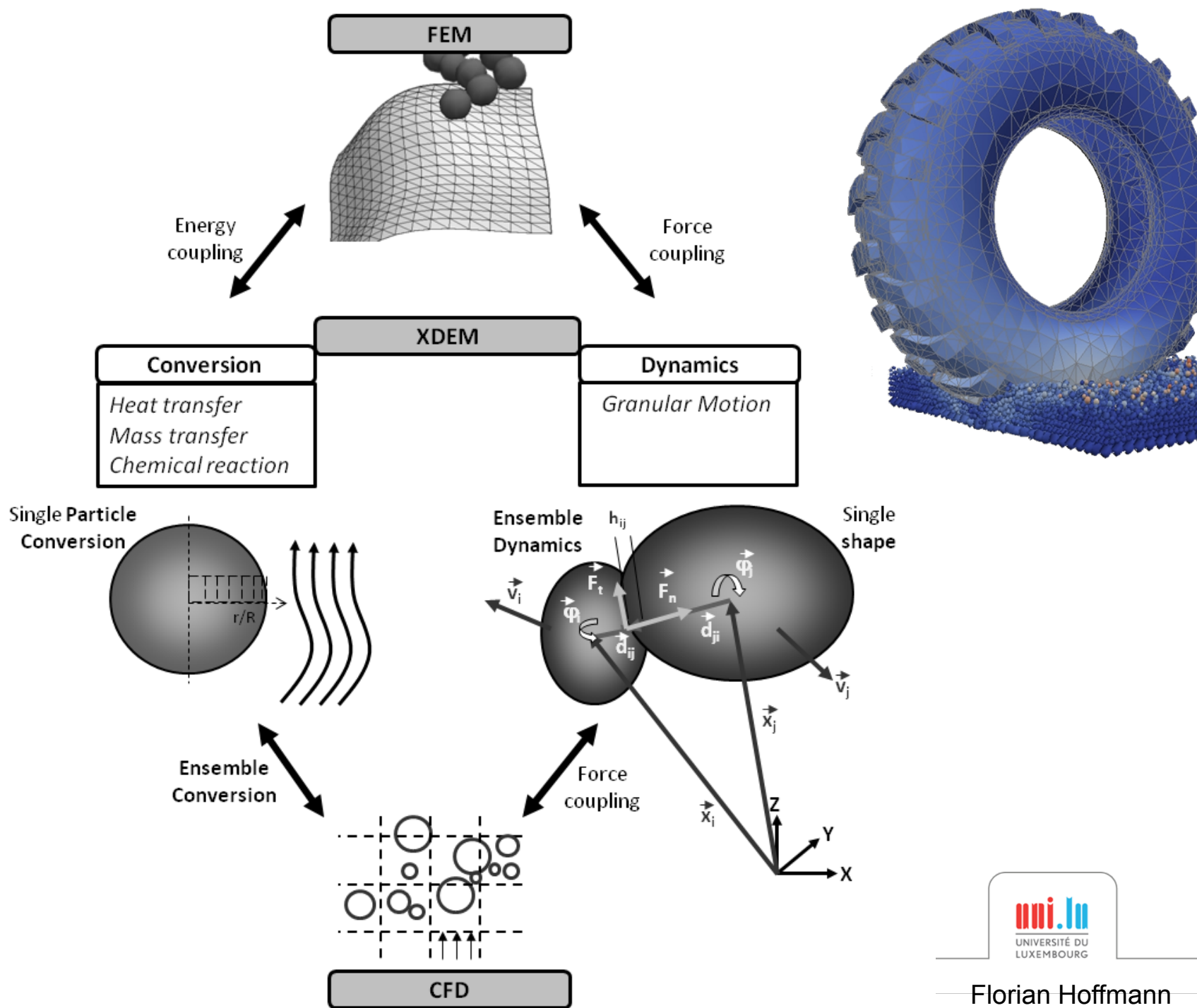


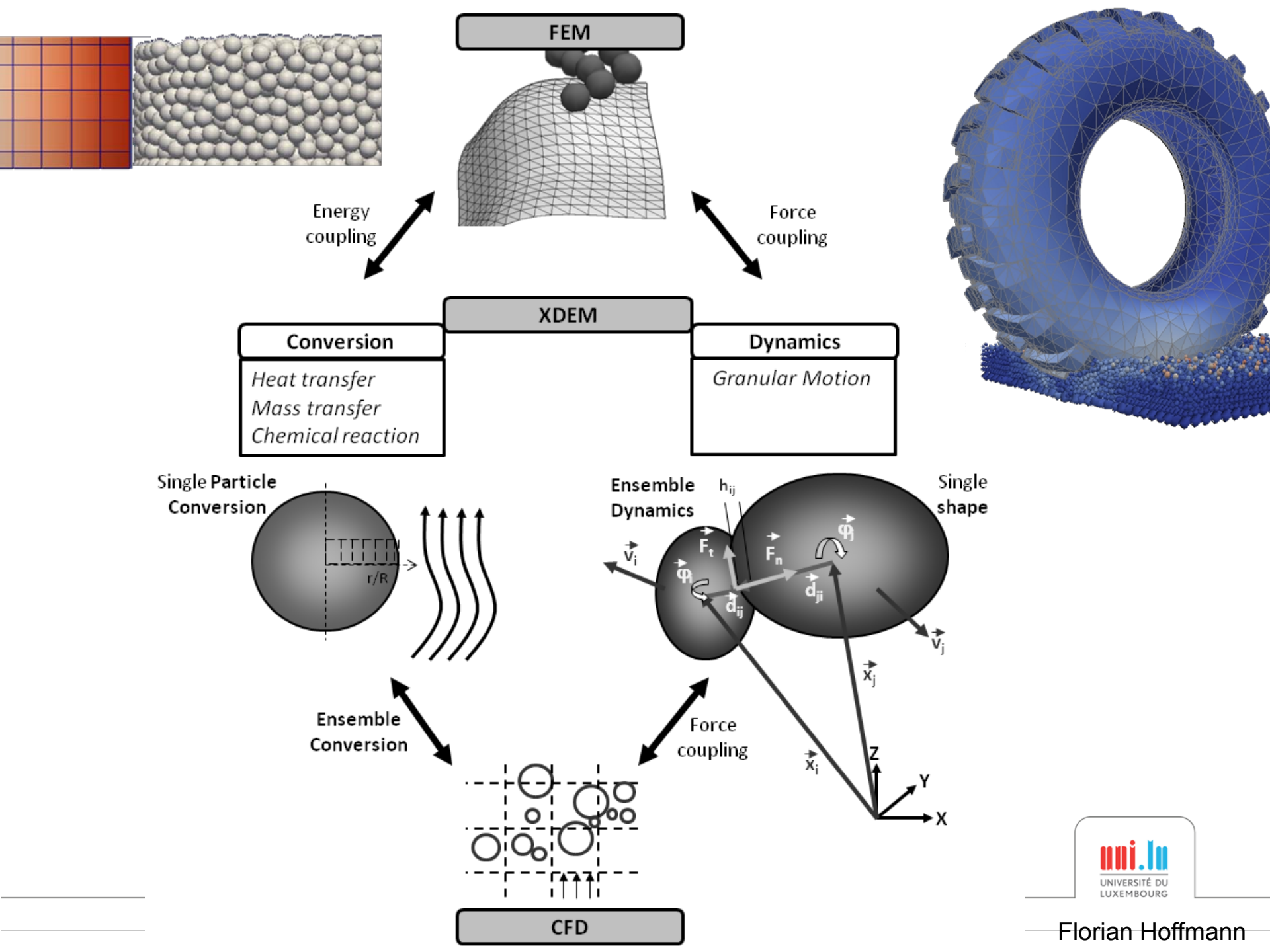
Chemische Prozesse

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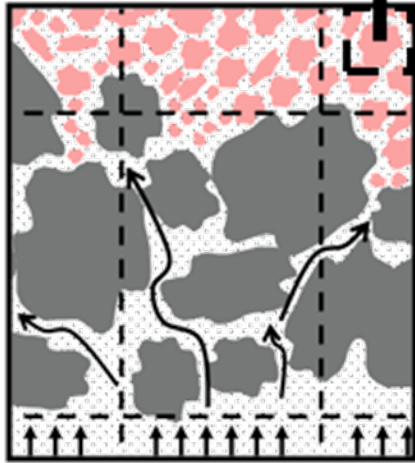
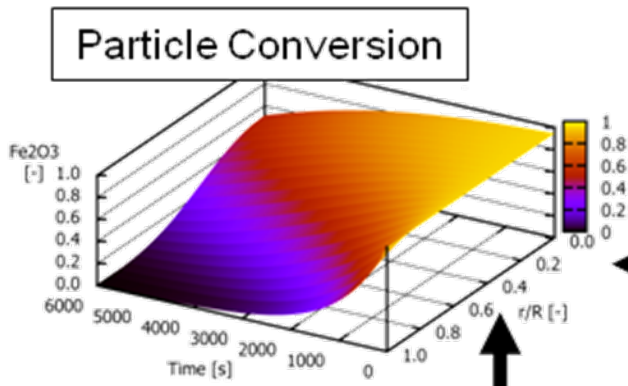




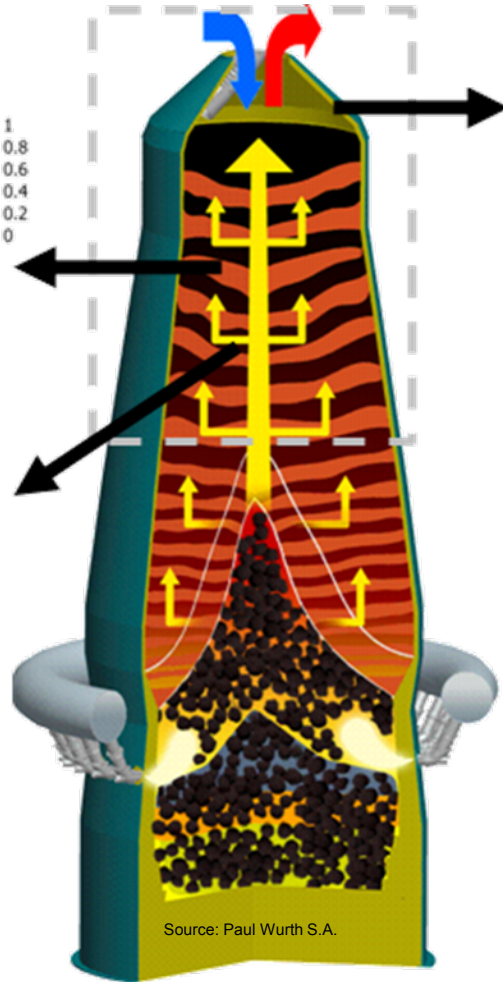




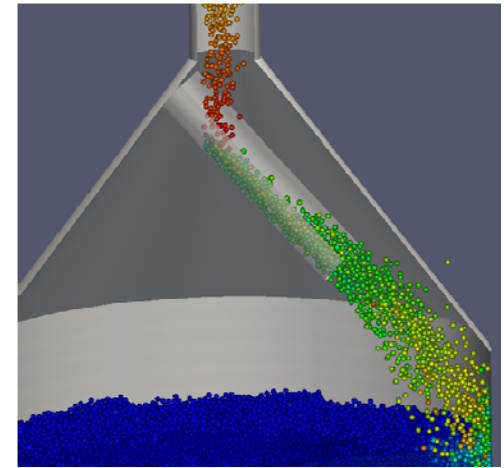
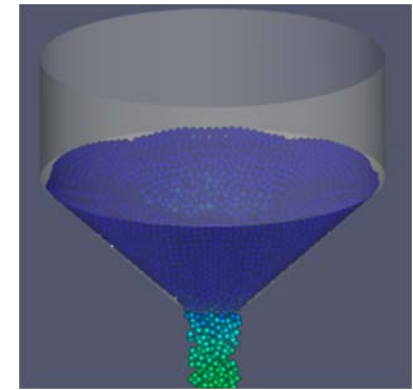
XDEM HO Schachtprozesse



Fluid flow



Source: Paul Wurth S.A.



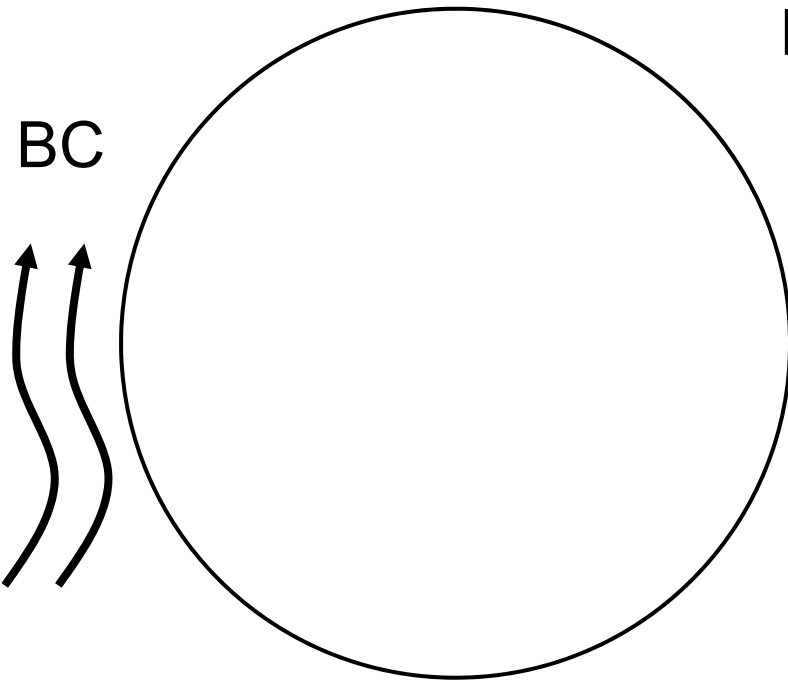
Particle Motion

XDEM Conversion – Einzelpartikelmodell

Partikel
(z.B. Fe_xO_y)

Partikelmodell der
thermochemischen Umsetzung mittels
PDGL für:

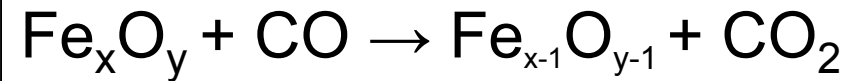
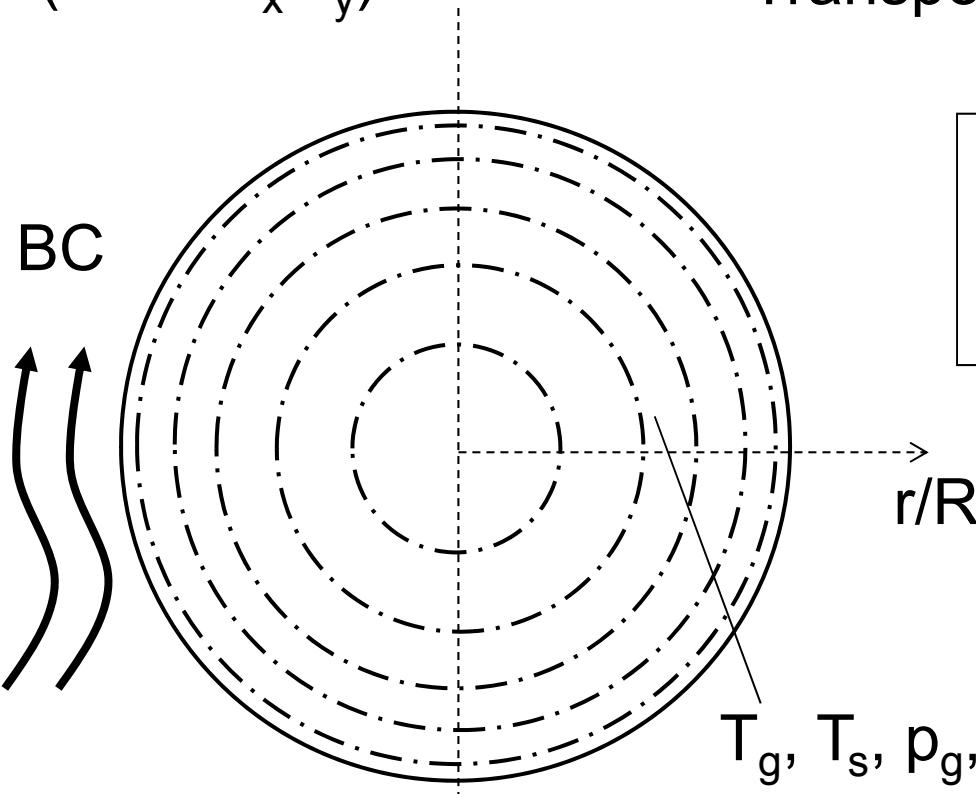
- Masse
- Spezies
- Energie



XDEM Conversion – Einzelpartikelmodell

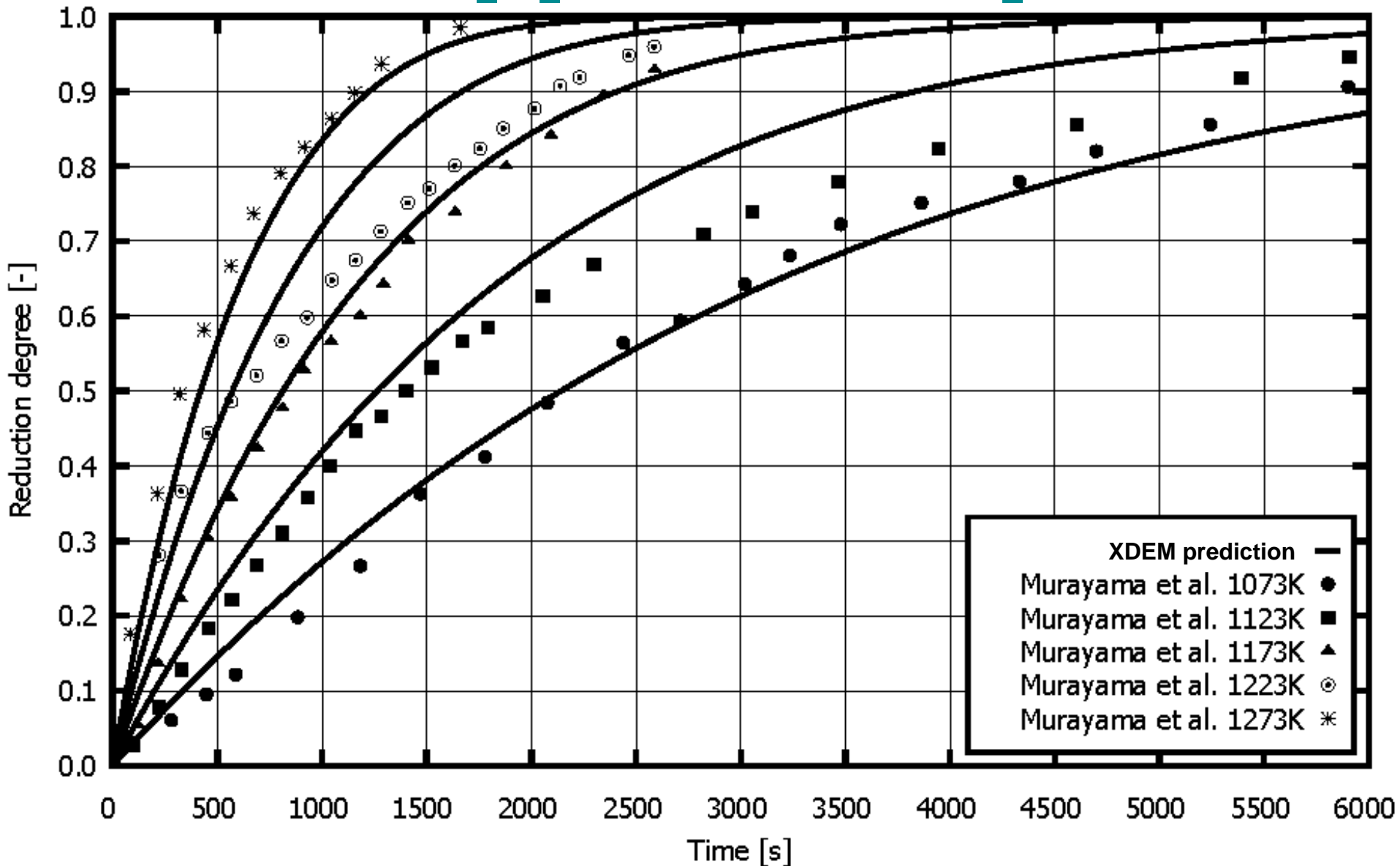
Partikel
(z.B. Fe_xO_y)

Transportprozesse und Reaktionskinetik

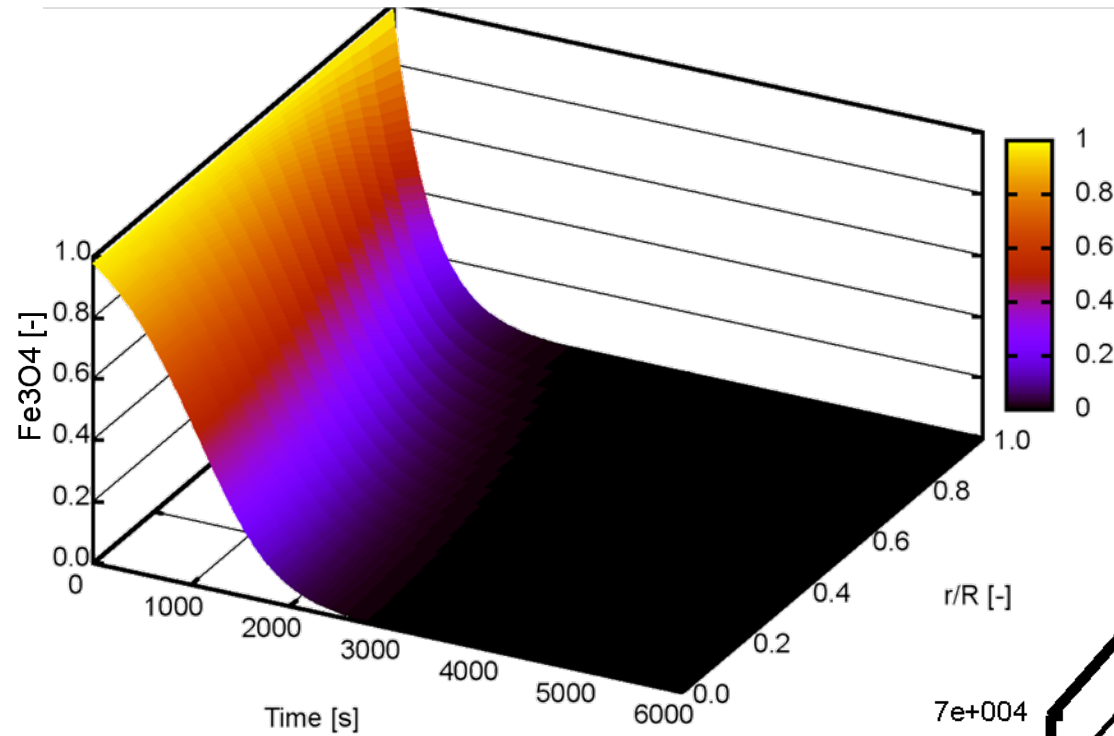


$$k(T) = k_0 * \exp(E_a/RT)$$

Validierung: $\text{Fe}_3\text{O}_4 + \text{CO} \rightarrow 3\text{FeO} + \text{CO}_2$ (isotherm)

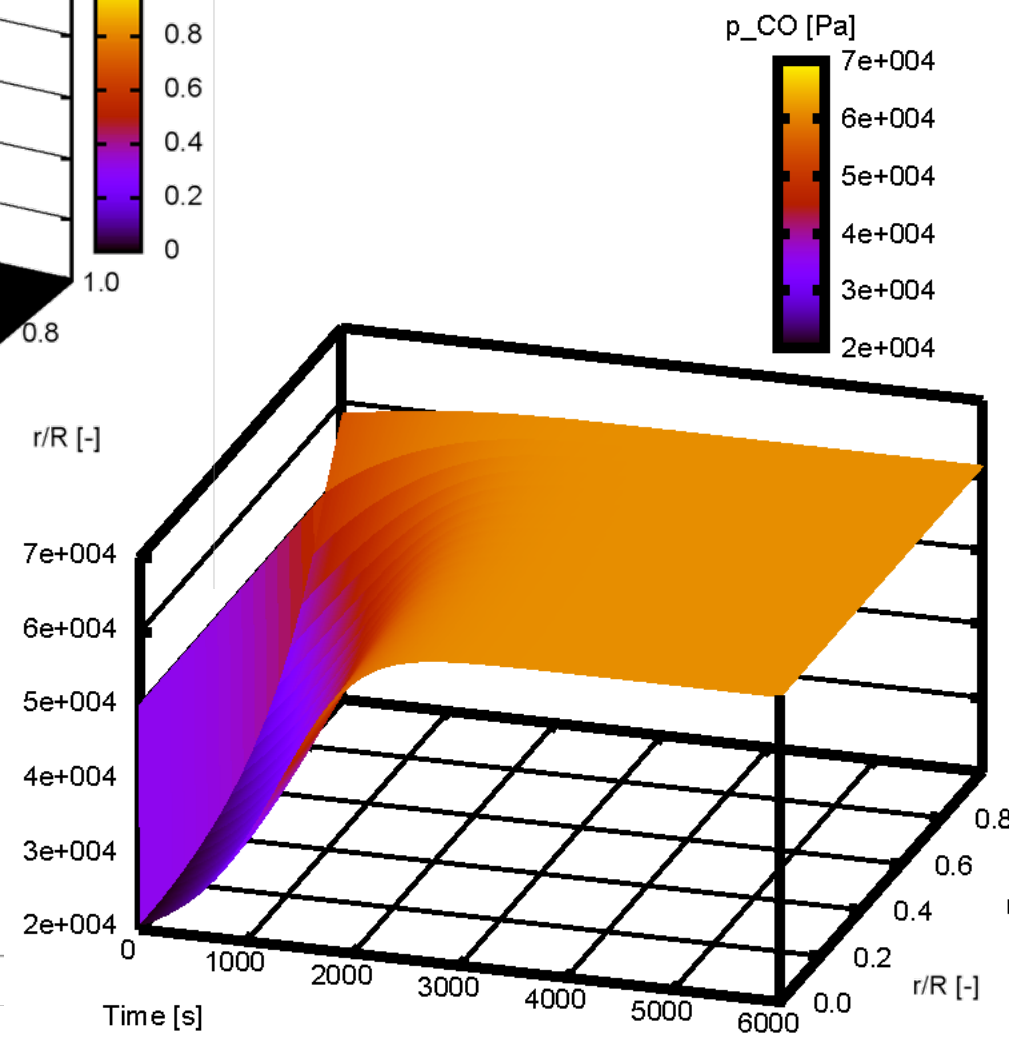


Validierung: $\text{Fe}_3\text{O}_4 \rightarrow \text{FeO}$ (1273 K)

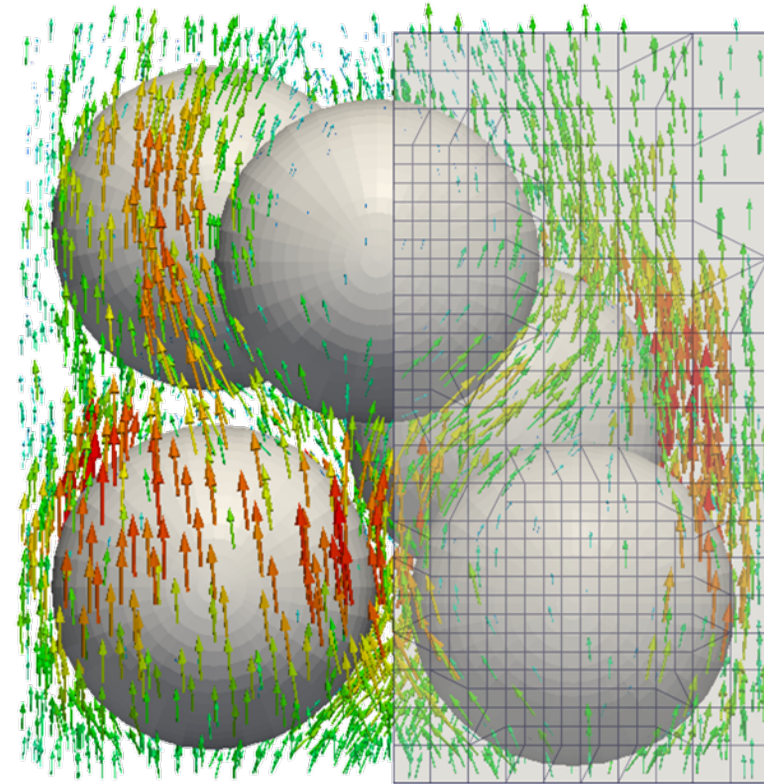
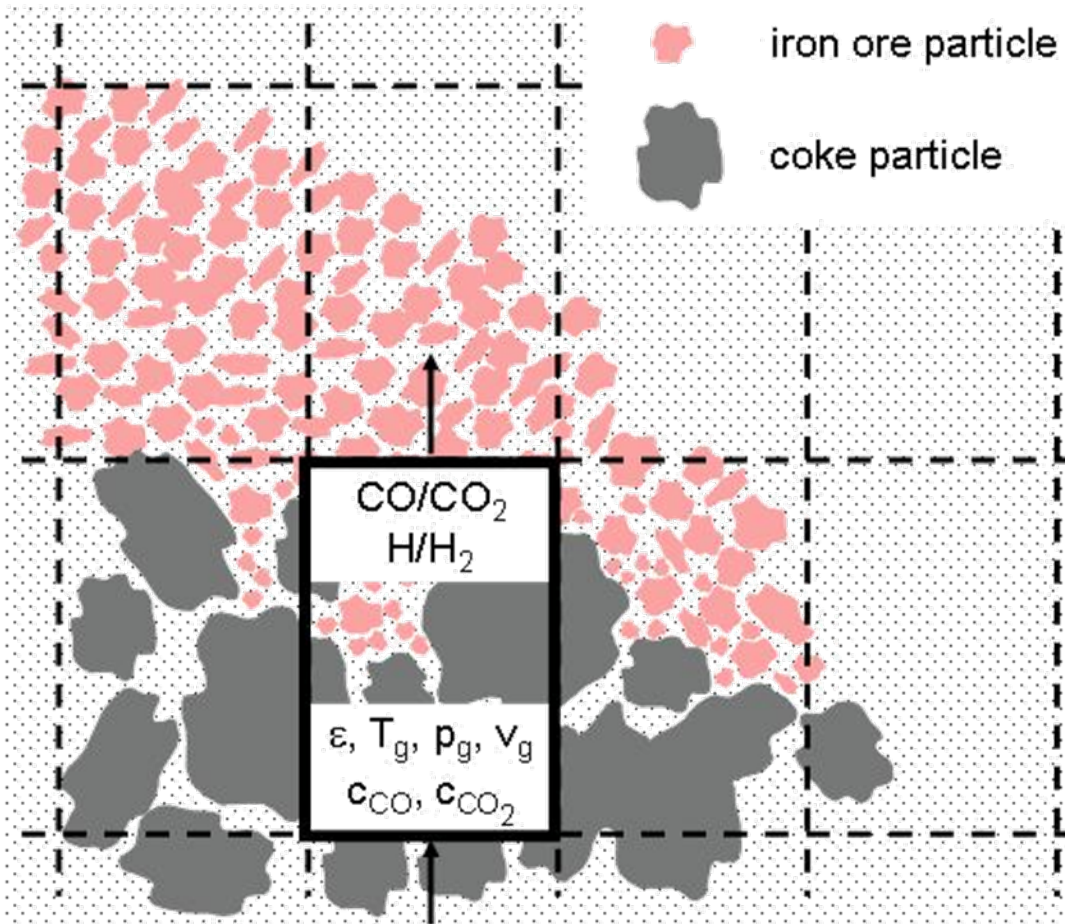


Massenanteil Fe_3O_4

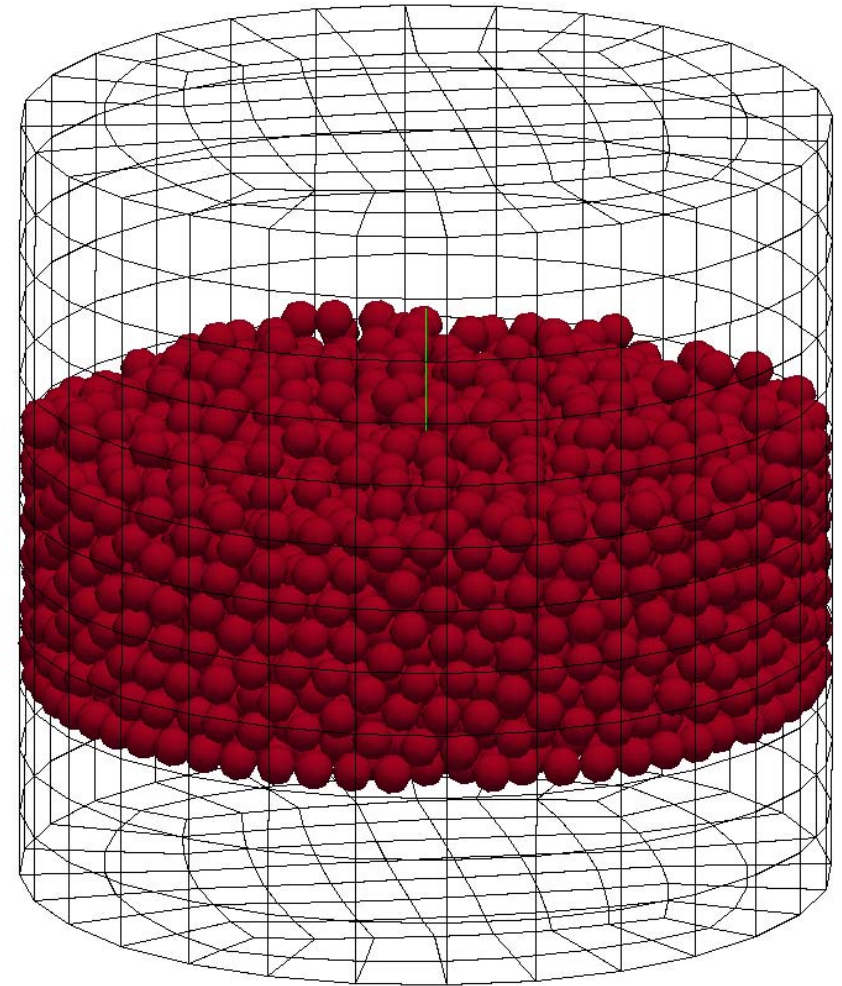
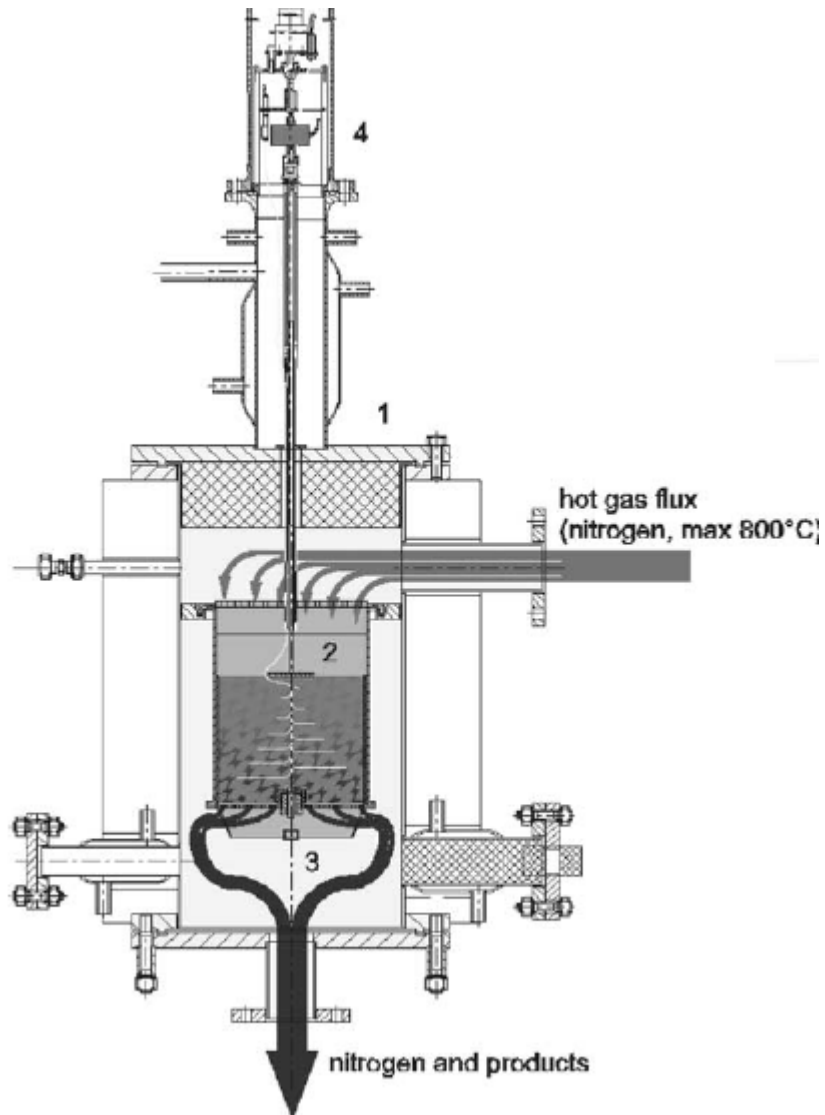
Partialdruck CO



XDEM Conversion, Festbettmodell

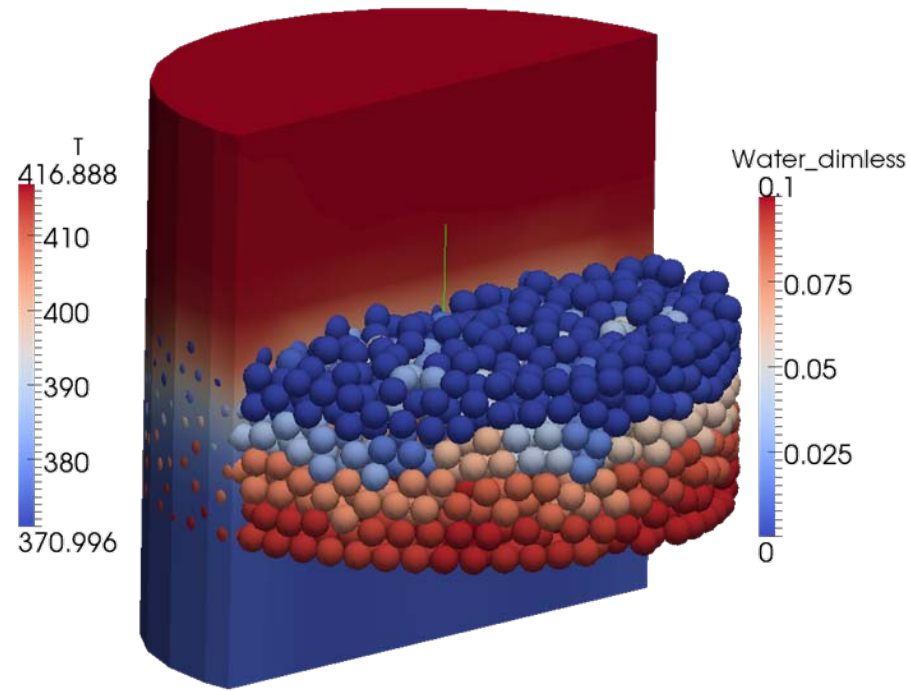
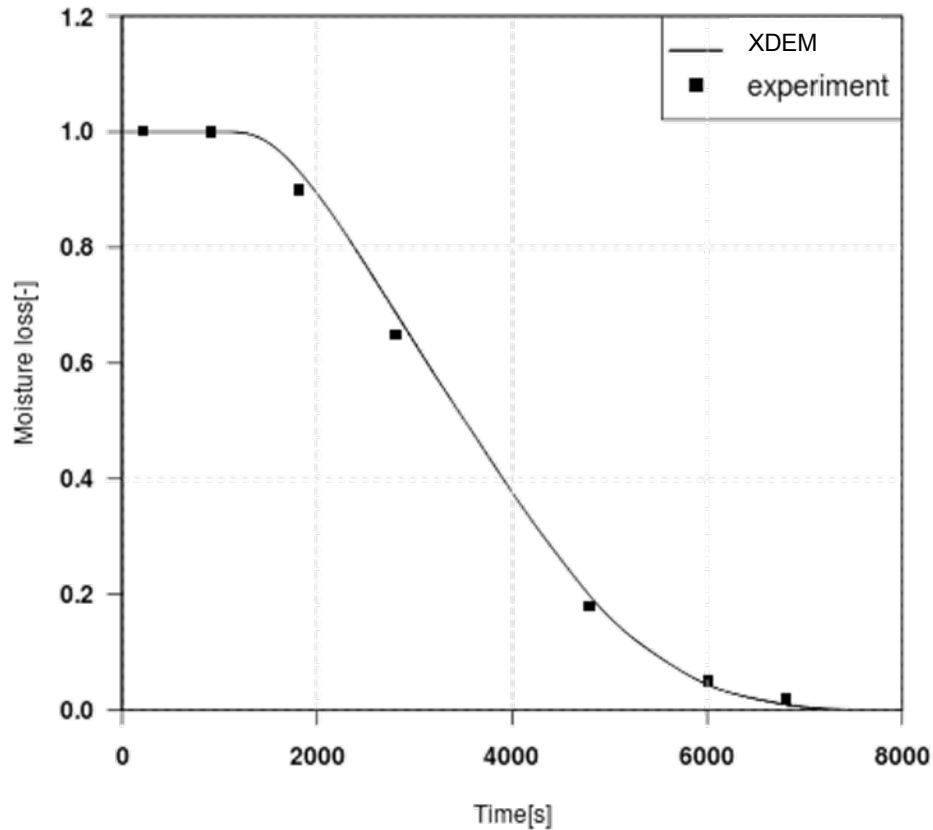


XDEM Conversion, Validerung des Wärme- & Stofftransports durch Experimente



XDEM Conversion, Holztrocknung

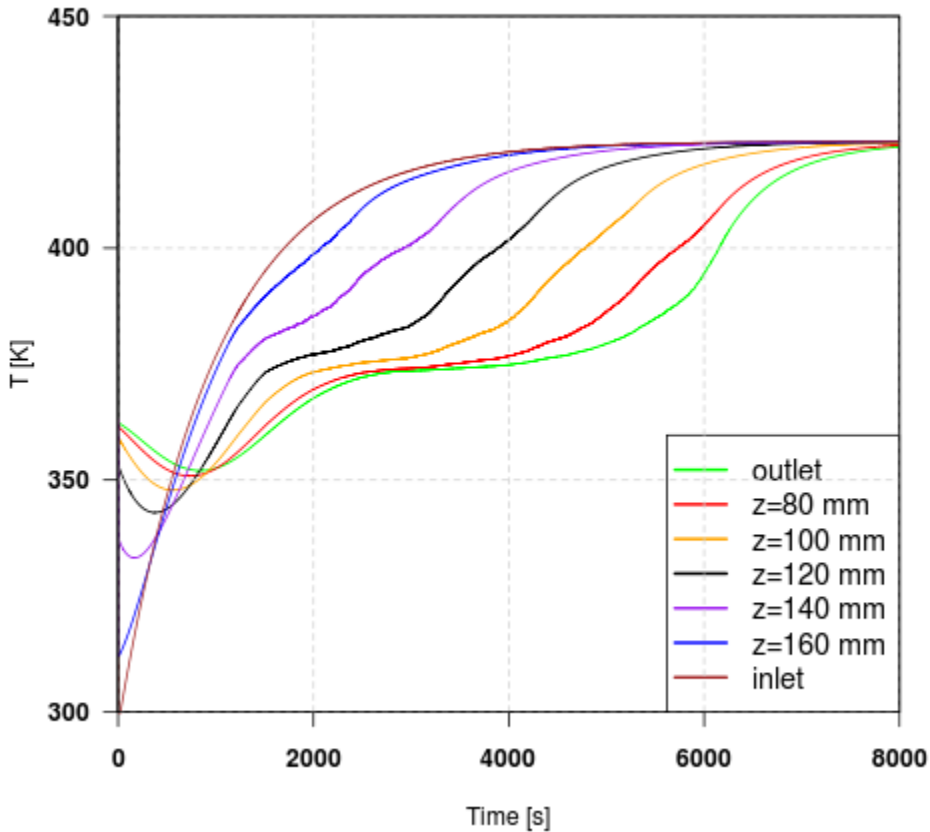
moisture loss at inlet temperature of 150 degree



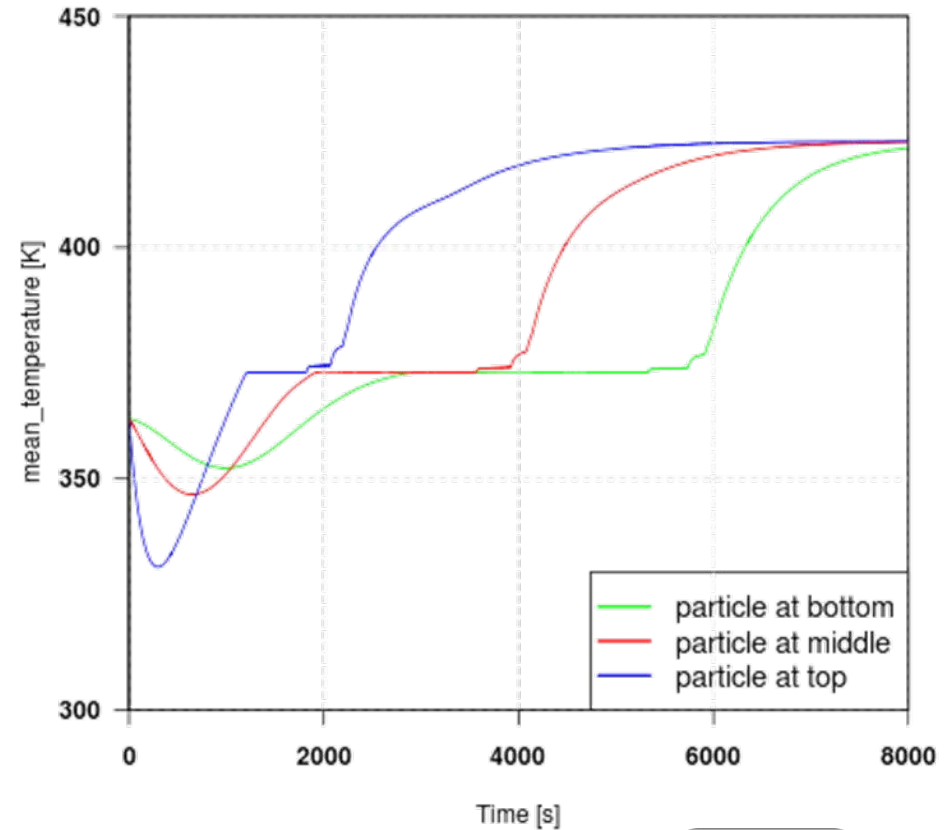
$t = 3000s$

XDEM Conversion, Detailansicht Einzelpartikel

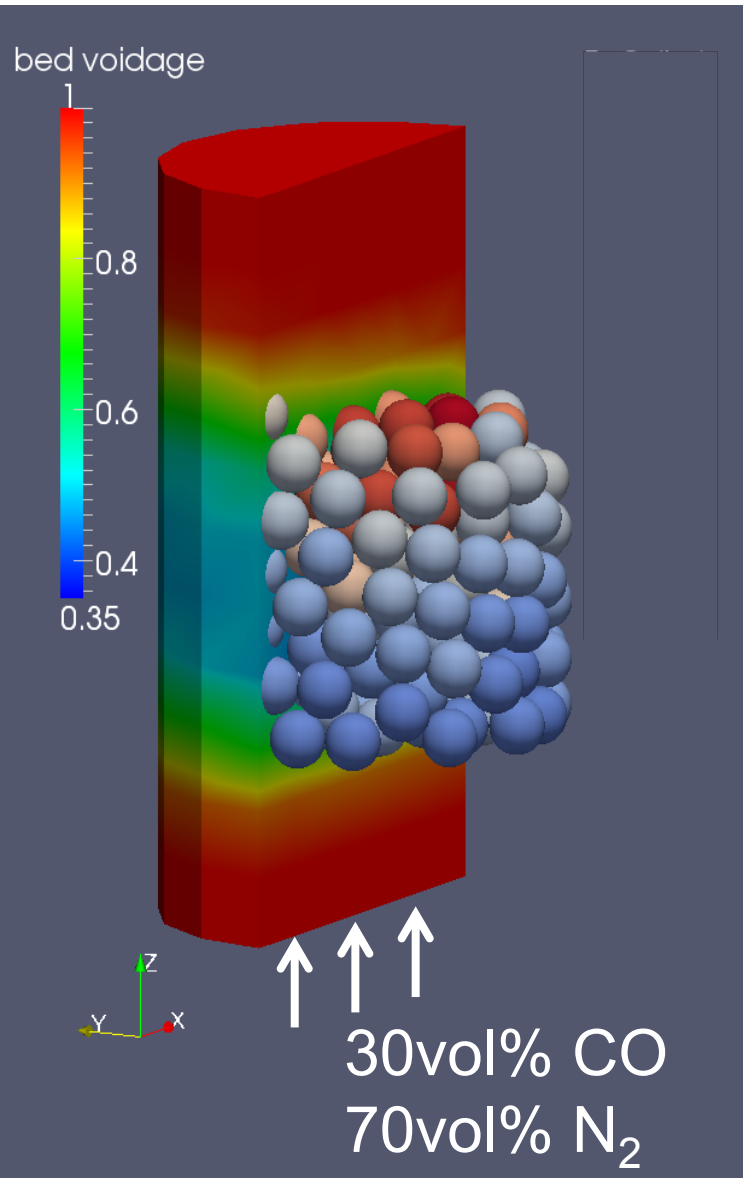
temperatures at different heights



mean temperature of particle at different height



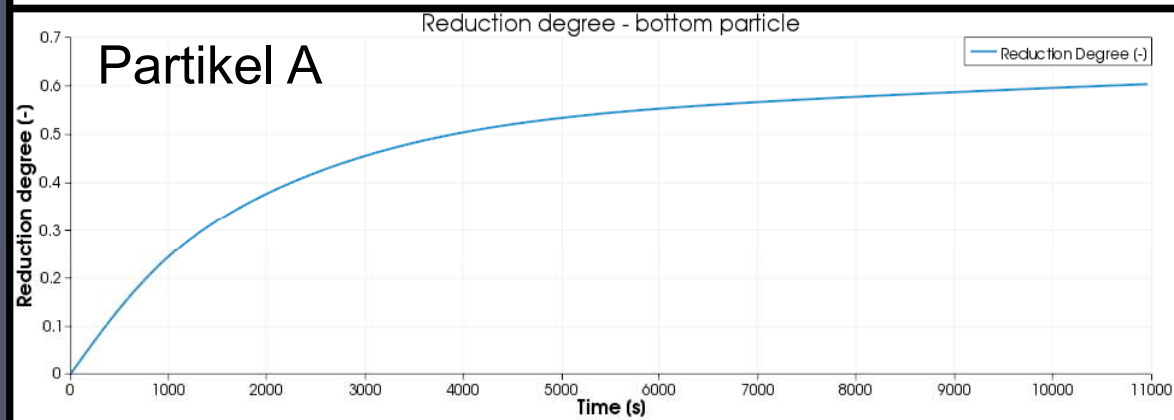
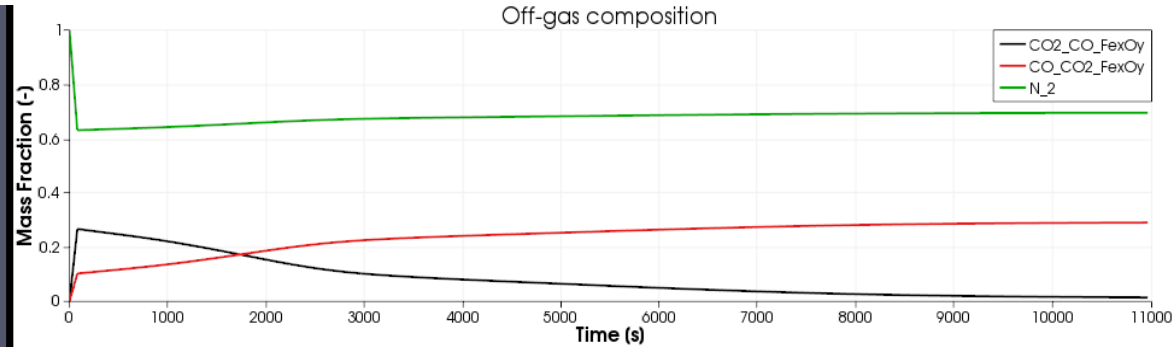
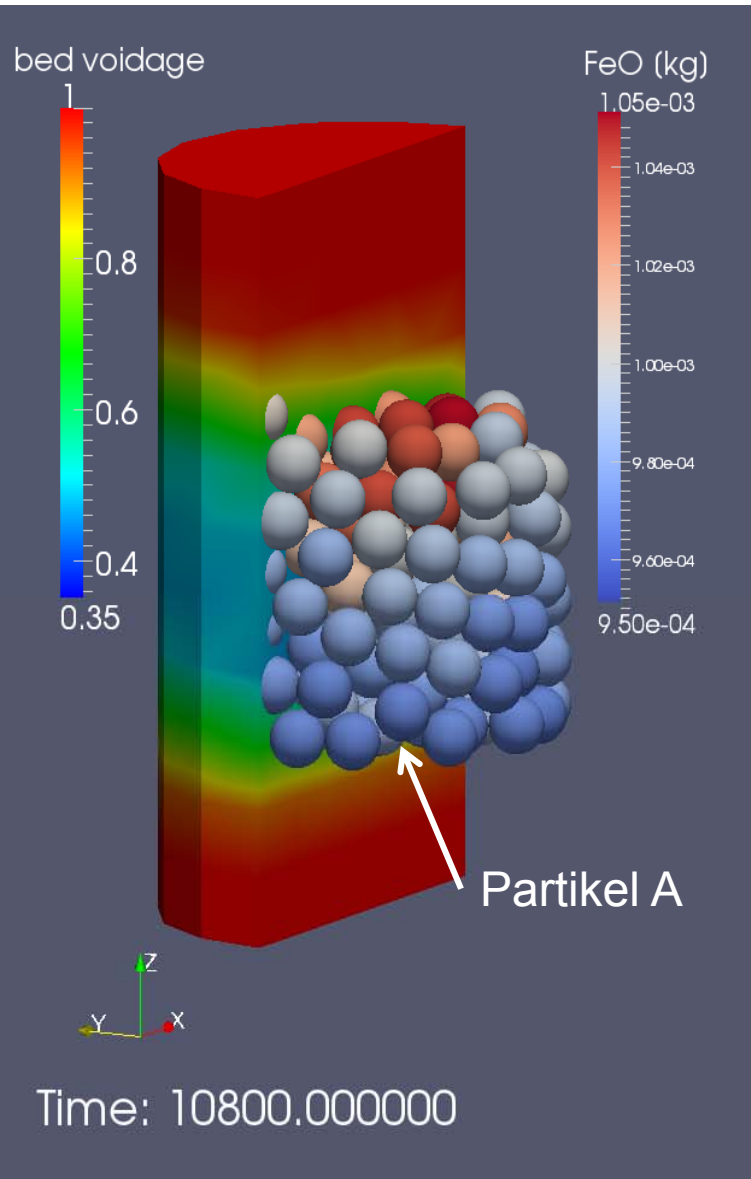
XDEM Conversion, Reduzierbarkeit ISO7215



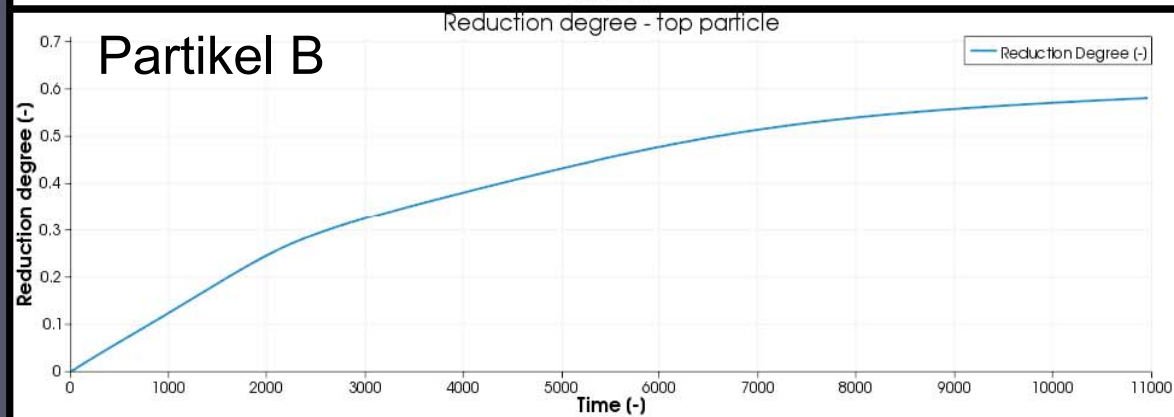
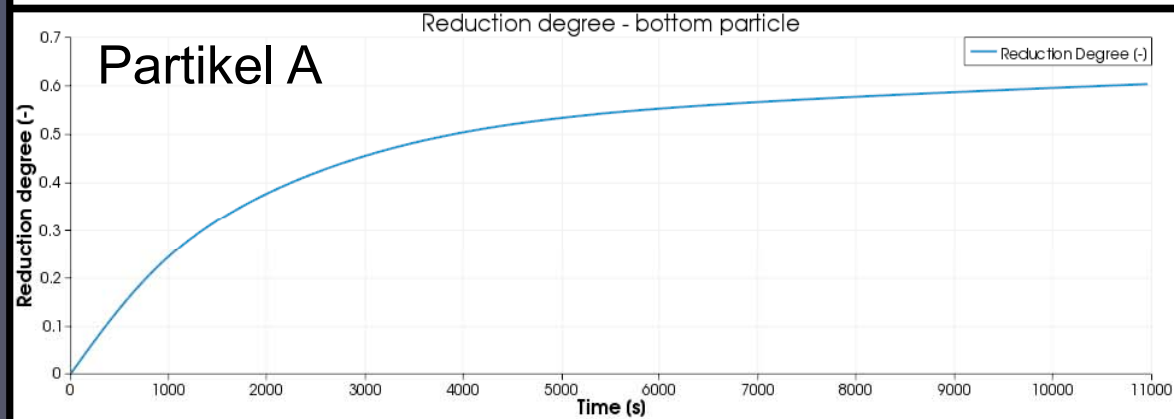
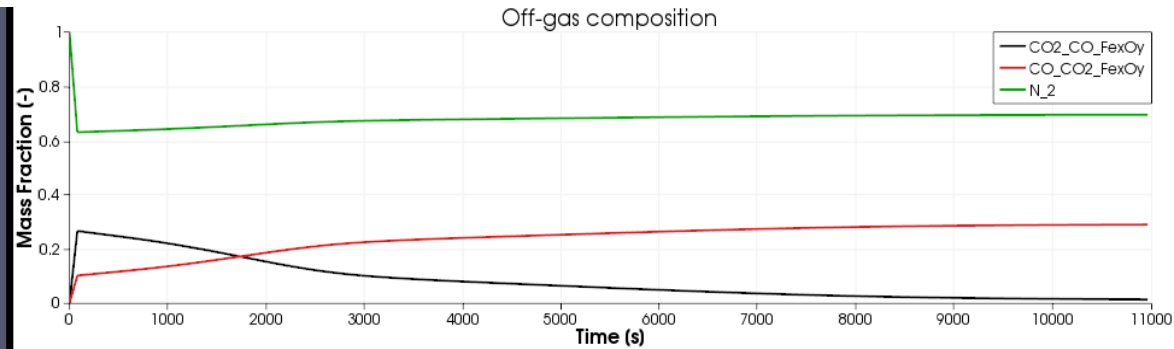
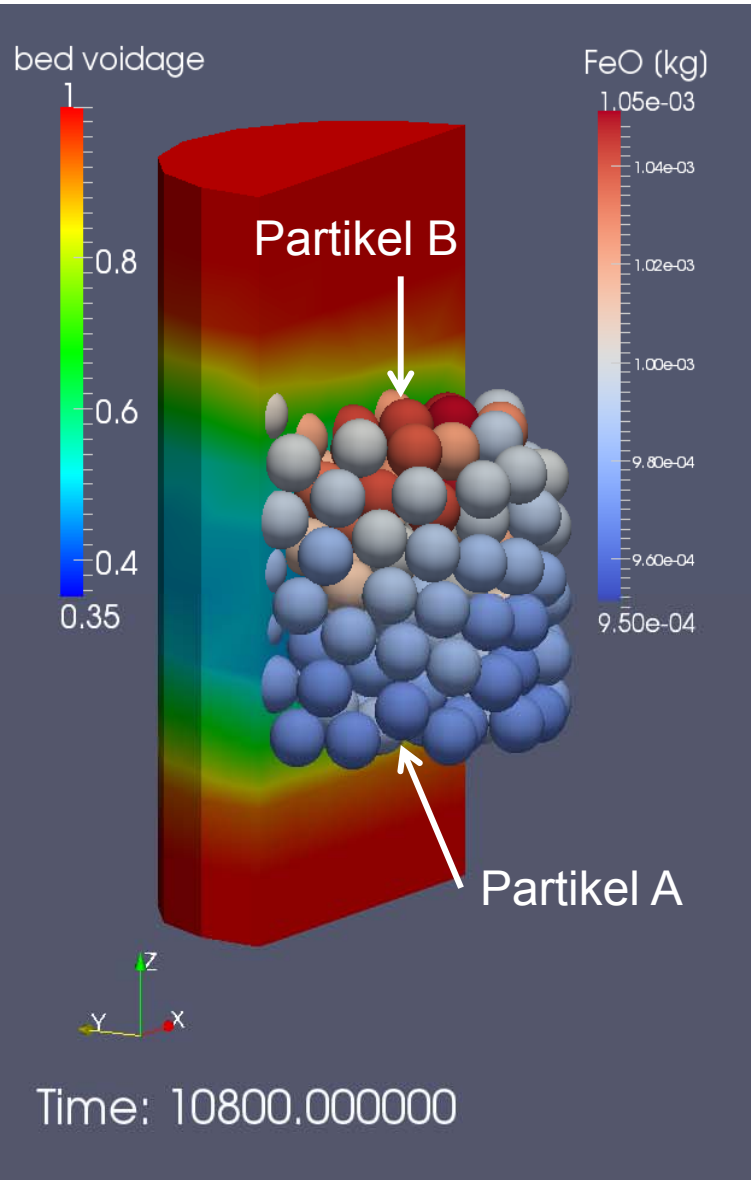
Reduzierbarkeitstest:

- 500 g Eisenerzpellets
- Indirekte Reduktion
 - 900°C
 - 15NI/min (CO/N₂ - Gemisch)
- -> Reduktionsgrad nach 180 min (R₁₈₀)

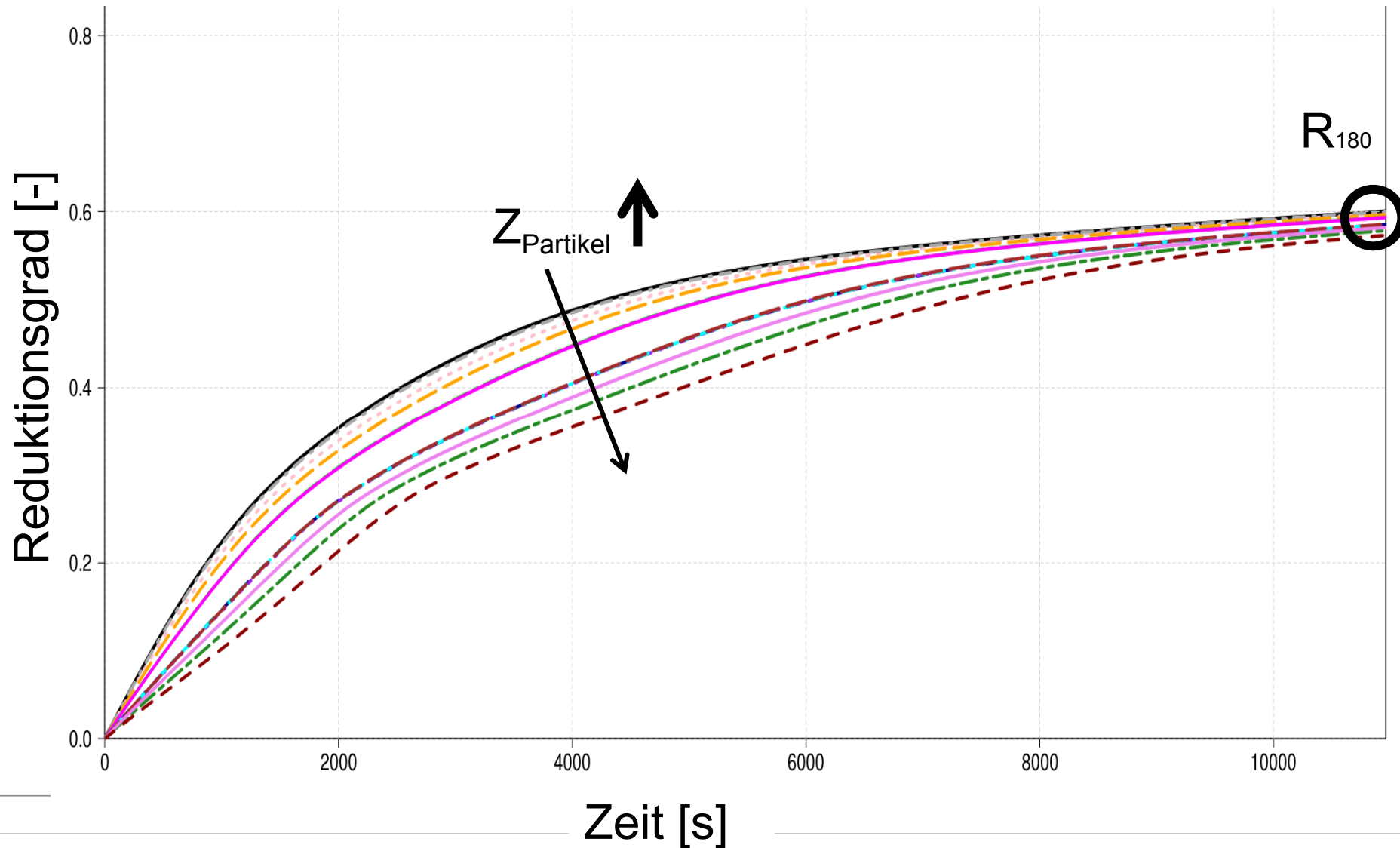
XDEM Conversion, Reduzierbarkeit ISO7215



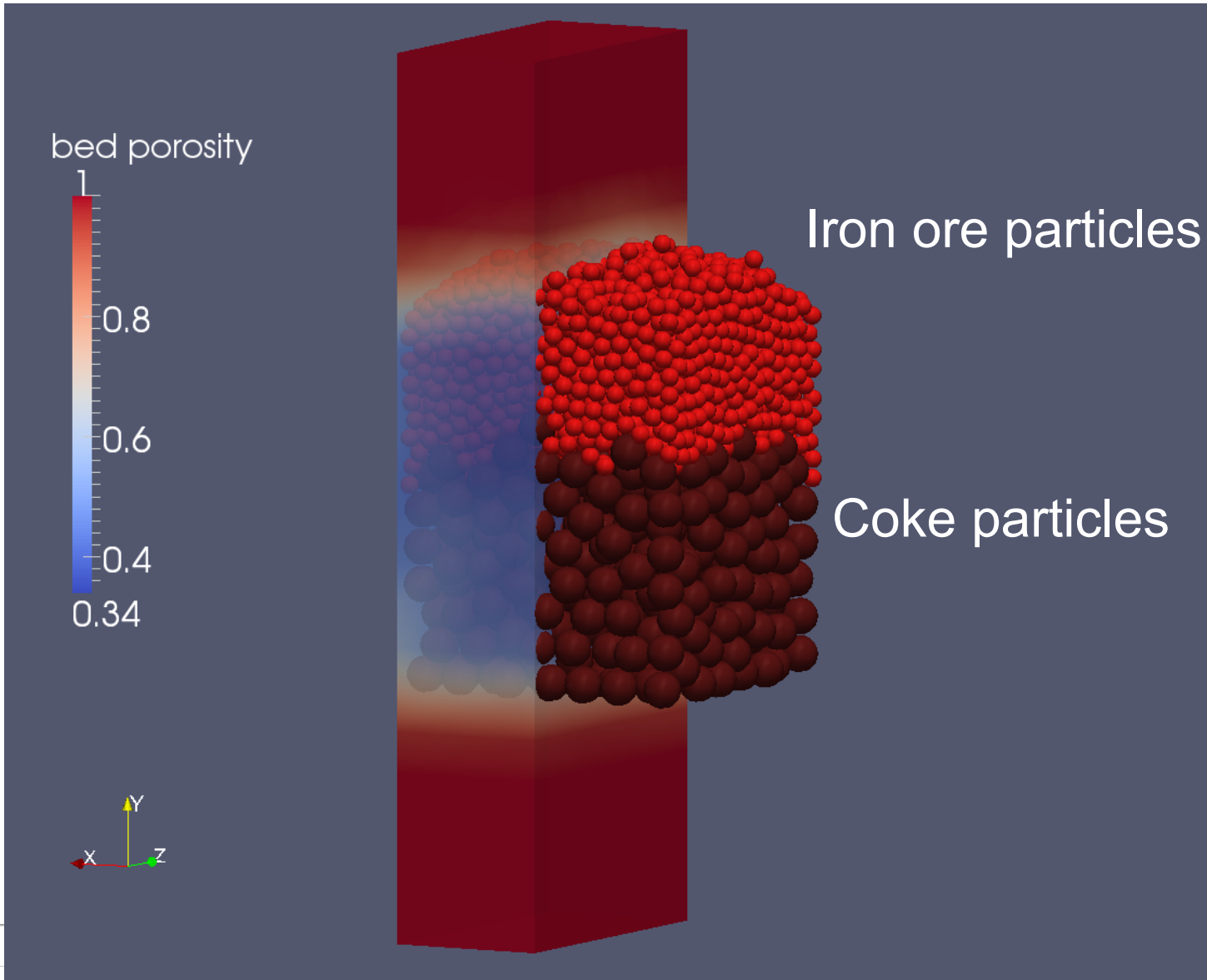
XDEM Conversion, Reduzierbarkeit ISO7215



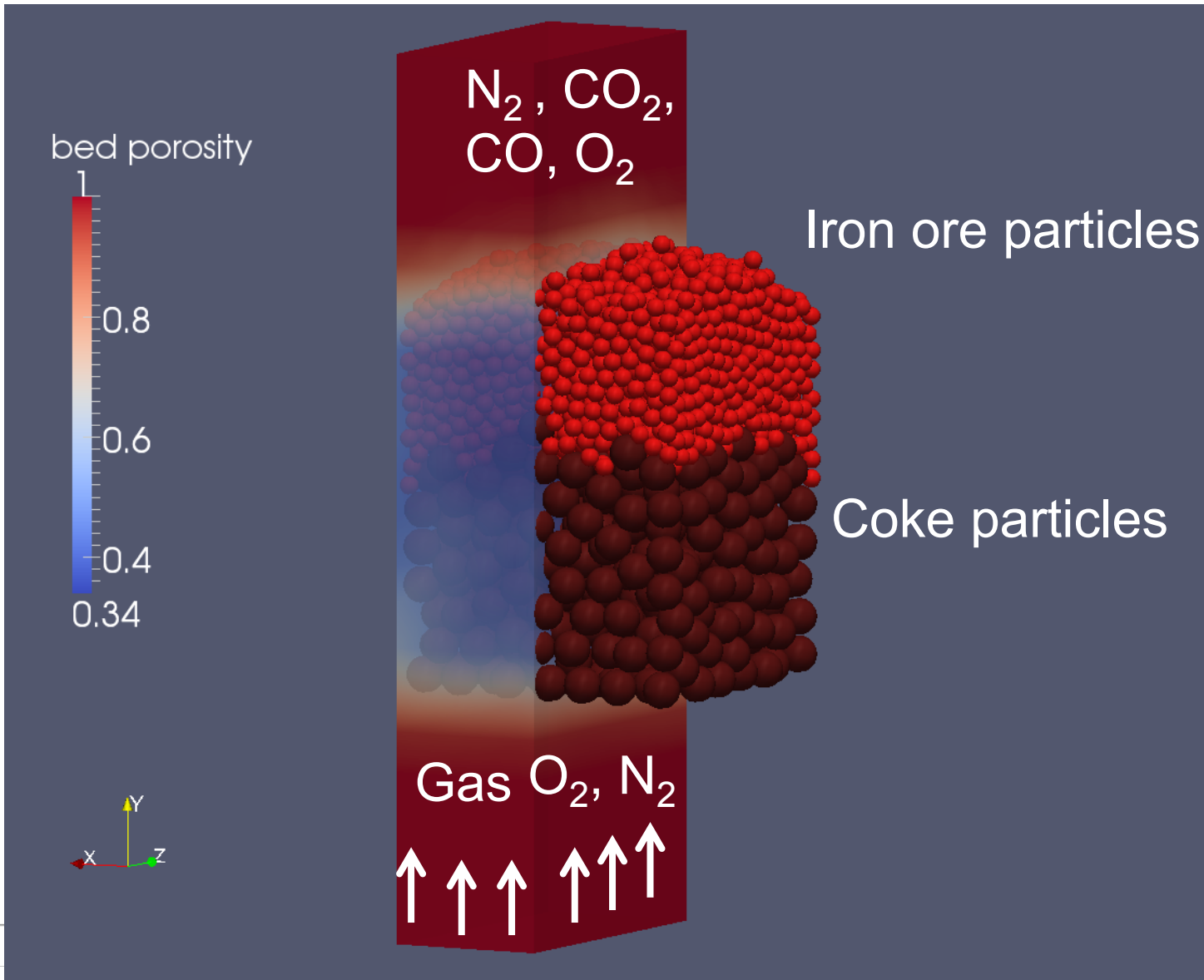
XDEM Conversion, Reduzierbarkeit ISO7215



Indirekte Reduktion



Indirekte Reduktion



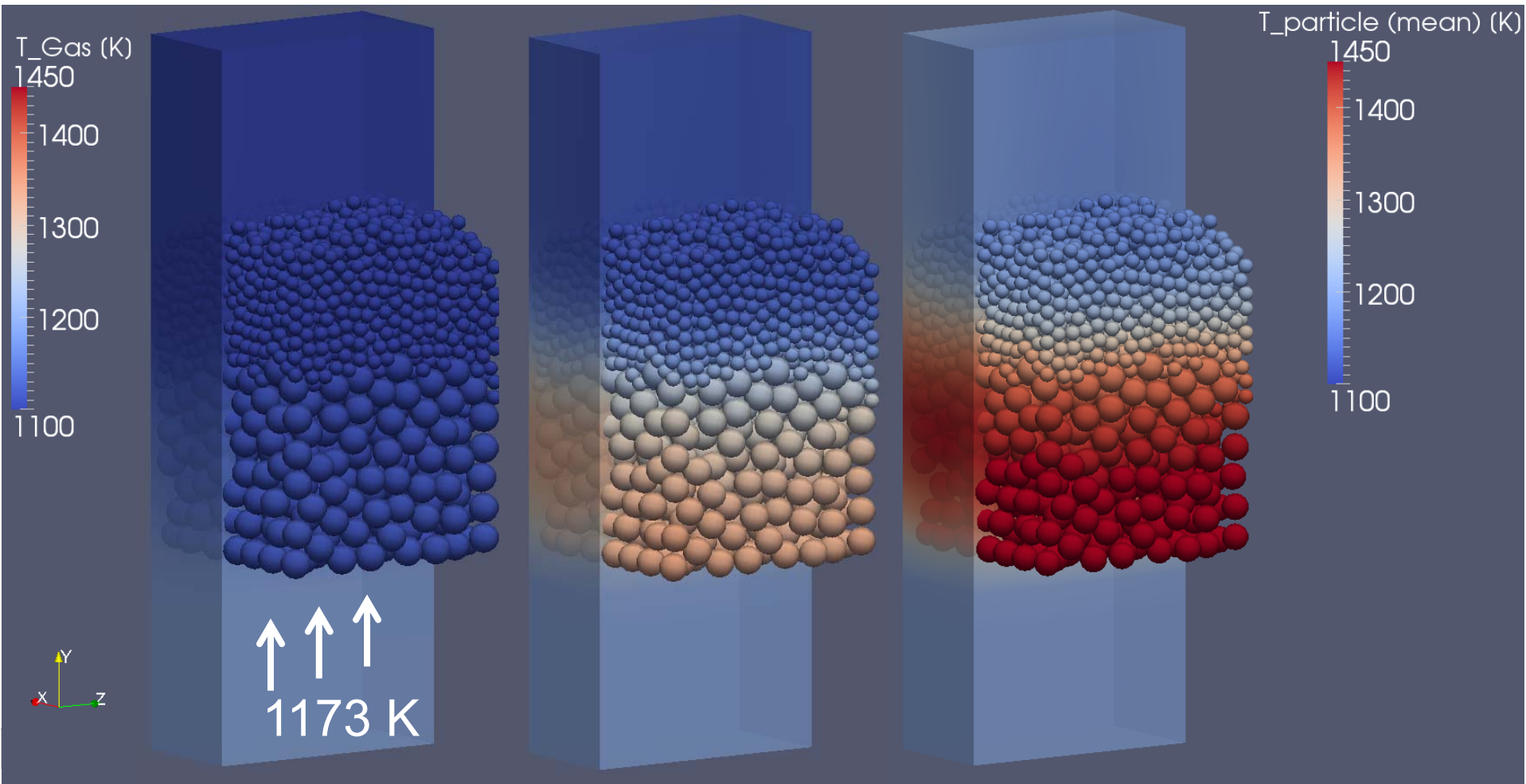
Indirekte Reduktion

$T_{\text{Inlet}}=1173 \text{ K}$

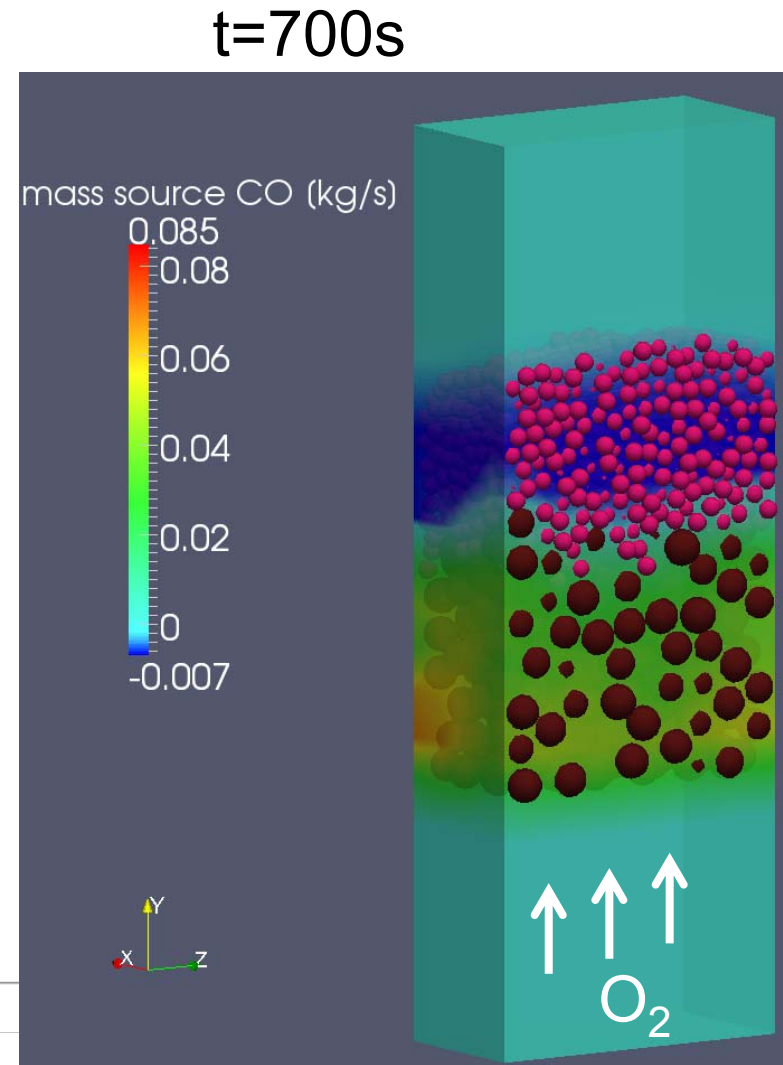
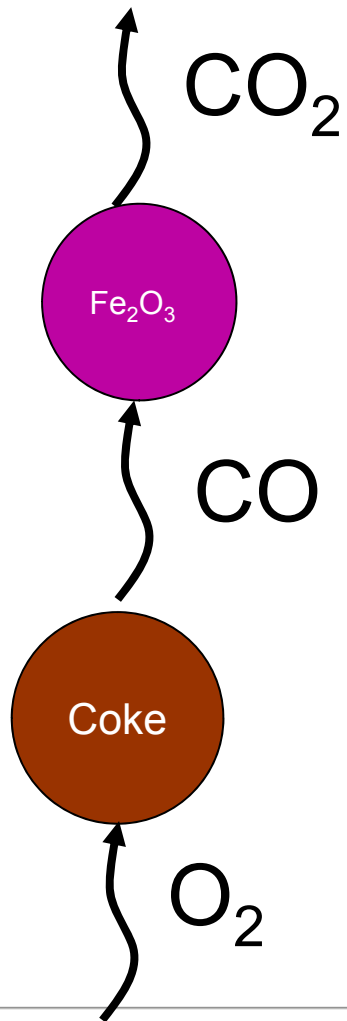
$t=10\text{s}$

$t=300\text{s}$

$t=700\text{s}$



Indirekte Reduktion

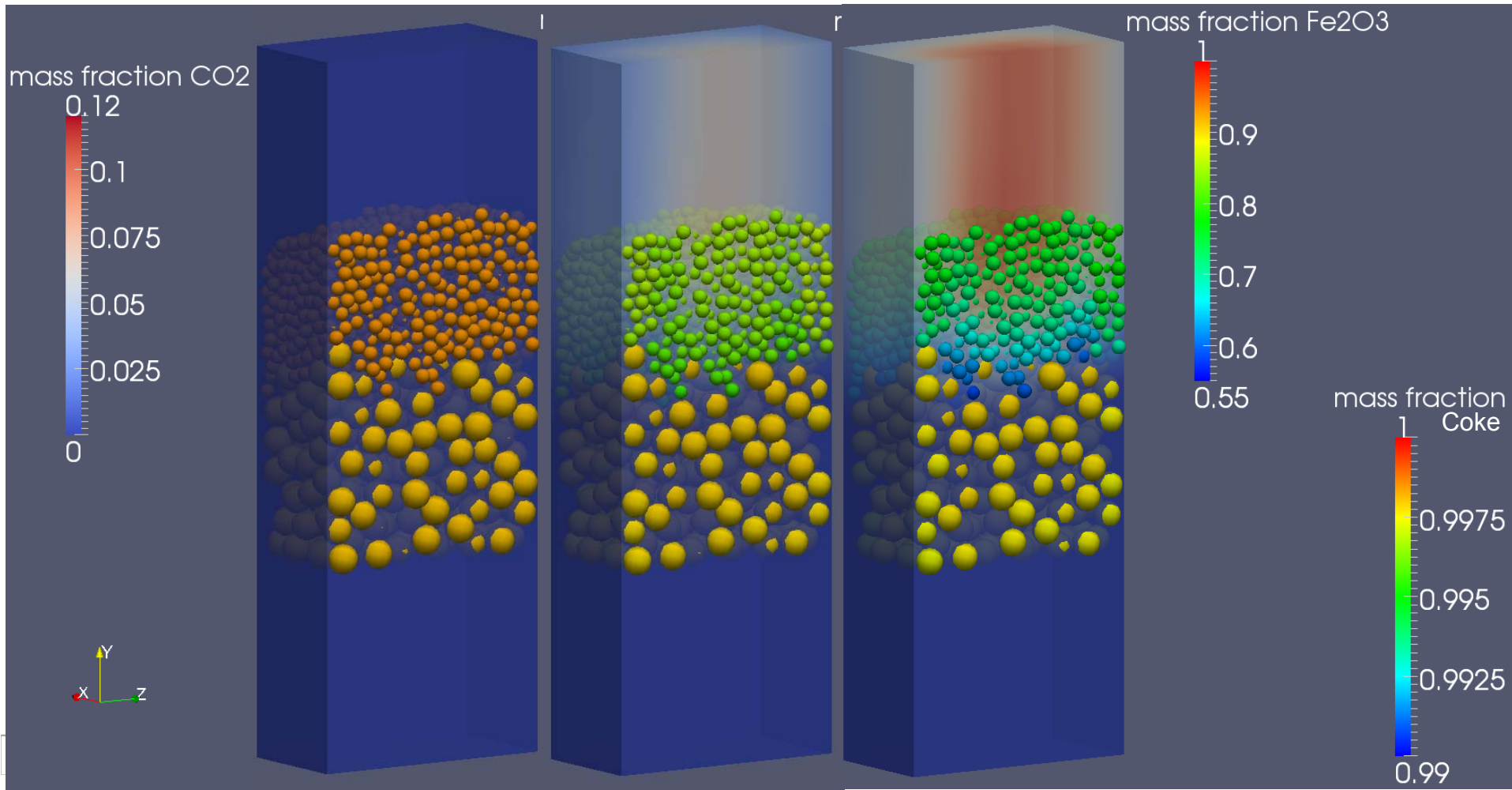


Indirekte Reduktion

t=10s

t=300s

t=700s



HO Modell

-Zonenmodellierung:

- Schaft
- Kohäsive Zone
- Blasform
- Herd
- ...

- 2D/3D

- 2/3/4 versch. Phasen

bed voidage

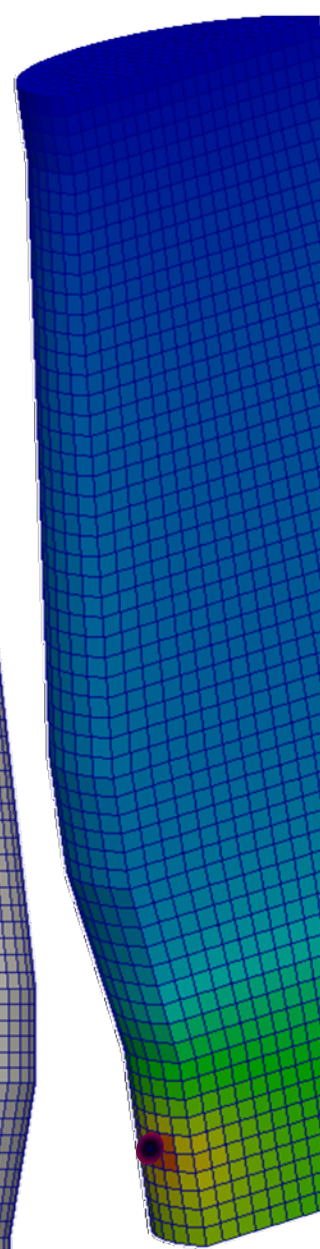
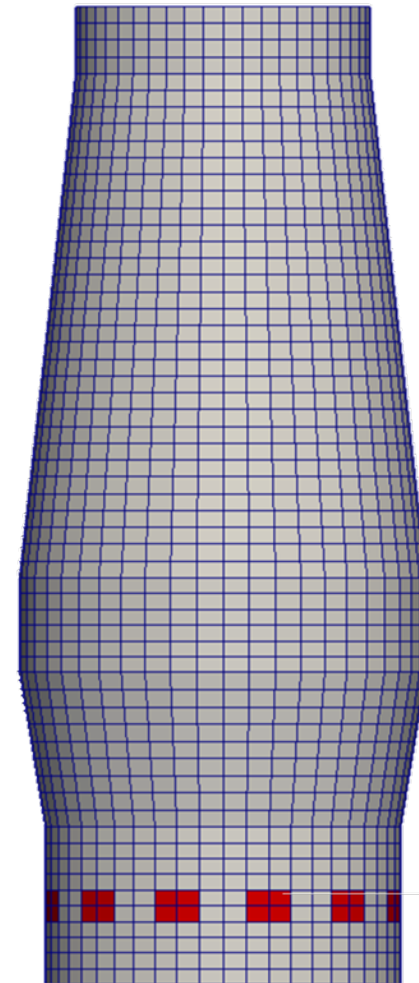
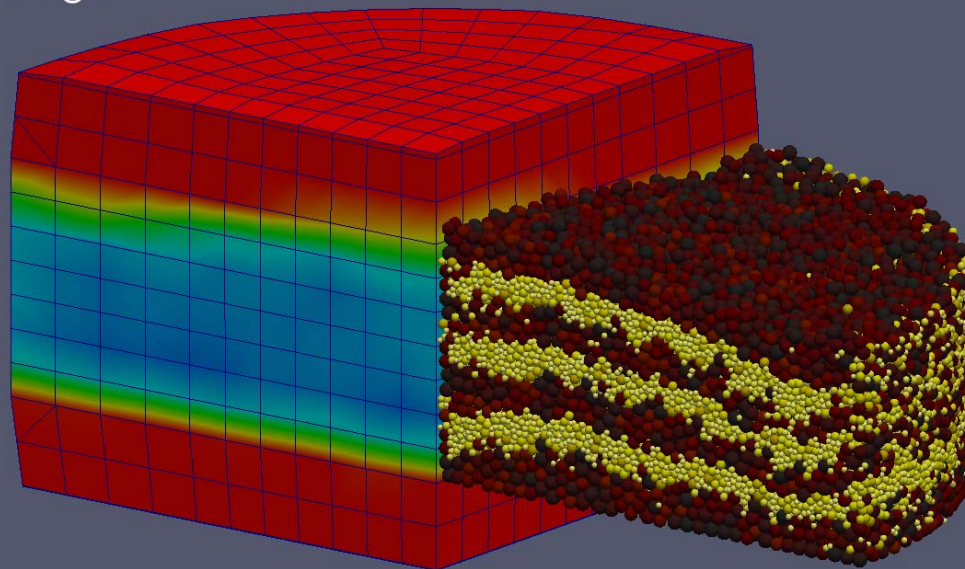
0.7

0.6

0.5

0.4

0.3



Conclusion

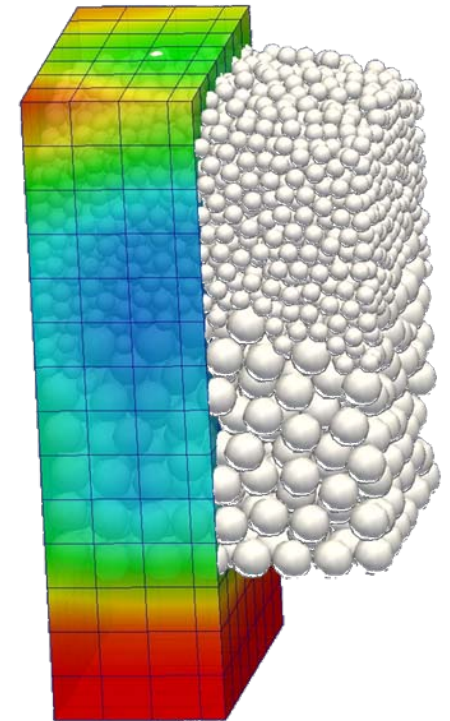
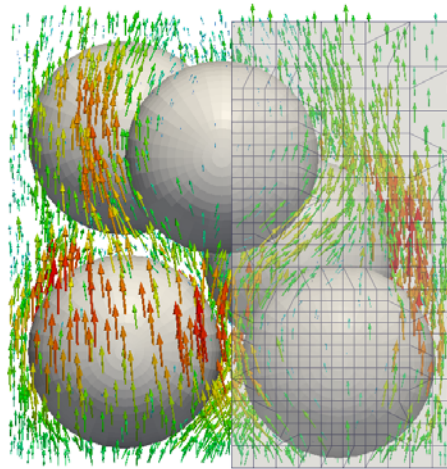
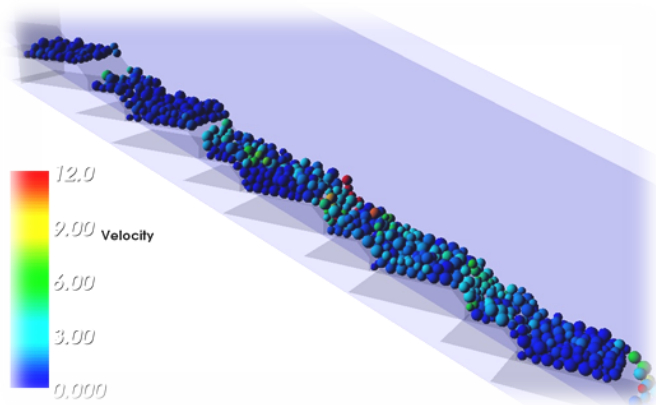
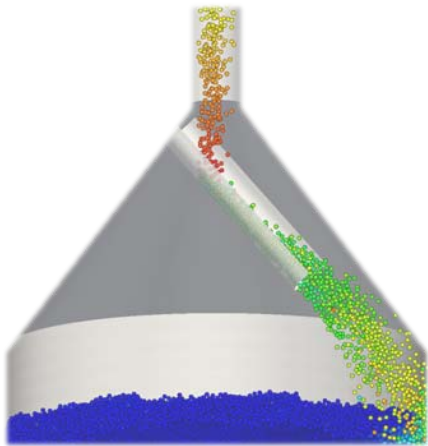
XDEM = Kopplung zwischen Diskretem und Kontinuumsansätzen zur Beschreibung Granularer Medien + thermochem. Prozesse:

- **Granulare Phase(n)**
- **Gas-/Flüssigphase(n)**
- **Thermochemischen Prozesse**
- **Prozessheterogenitäten**
- **Intrinsische Modellparameter (Diffusion, Kinetik, Lückengrade, ...)**

Thank you for your attention

Visit us at

www.xdem.de



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