Institute of Engineering Thermodynamics

# A Methodology to Investigate the Liquid-Gas Kinetics in Molten Nitrate Salt

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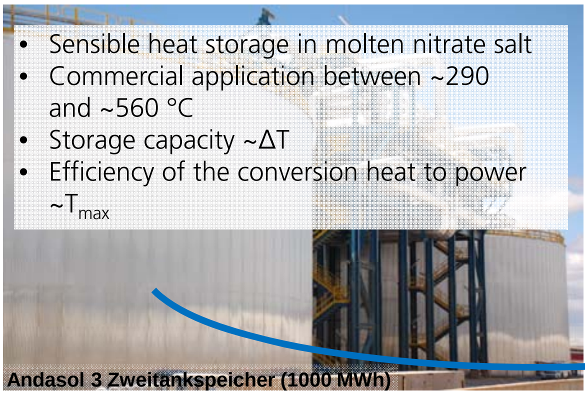
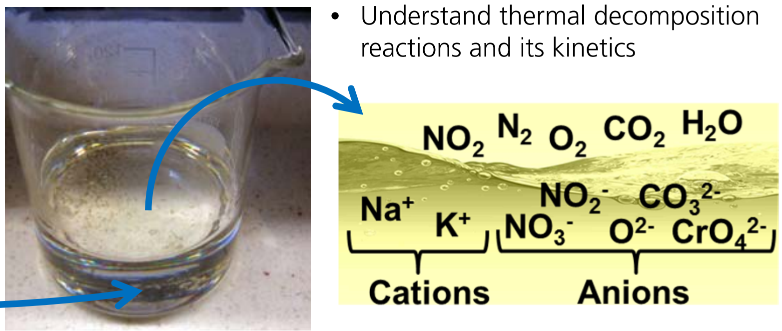
## Motivation

- Sensible heat storage in molten nitrate salt
- Commercial application between ~290 and ~560 °C
- Storage capacity ~ΔT
- Efficiency of the conversion heat to power ~$T_{max}$




## Goals

- Increase nitrate salt stability at high temperatures (>560 °C)
- Understand thermal decomposition reactions and its kinetics




## State of Knowledge

- Reversible reaction of nitrate ions forms nitrite ions and oxygen

$$NO_3^- \rightleftharpoons NO_2^- + 0.5\,O_2$$ ✓

$$\frac{d[NO_2^-]}{dt} = k_{Red} \cdot c_{NO_3^-} - k_{Ox} \cdot p_{O_2} \cdot c_{NO_2^-}$$

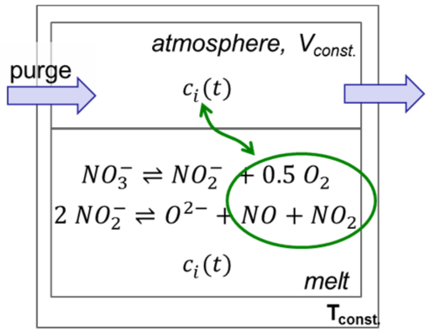
- Reactions that form nitrous gases $NO_x$, e.g.

$$2\,NO_2^- \rightleftharpoons O^{2-} + NO + NO_2$$ ?

$$v = k_{Dec} \cdot {c_{NO_2^-}}^2 - k_{Form} \cdot c_{O^{2-}} \cdot c_{NO} \cdot c_{NO_2}$$ ?

## Kinetic Modeling

- Calculates the time-dependent species concentrations of $NO_3^-$, $NO_2^-$, $O^{2-}$, $N_2$, $O_2$, $NO$, $NO_2$
- Assumptions
  - Instant equilibrium of dissolved and gaseous $O_2$ (Henry's law)
  - Constant in all directions in space (0D model)
  - Ideal liquid mixture/mixture of ideal gases
  - p, T=const.

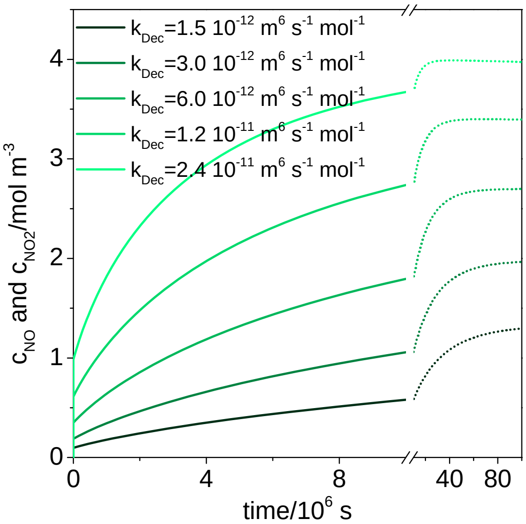



## Simulation Results

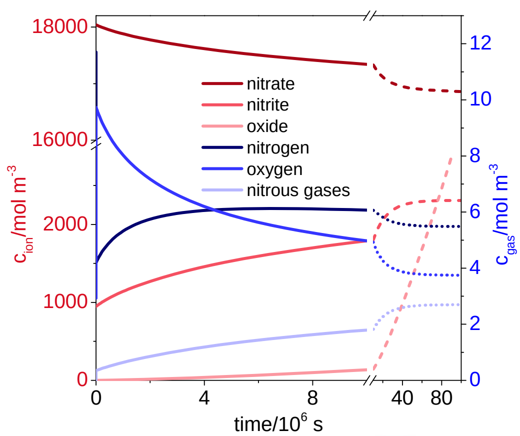
- Parametric sweep for the rate constants of the $NO_x$ forming reaction

Simulation conditions

- Initial ion ratio $c_{NO_2^-} / c_{NO_3^-} = 5 / 95$
- Initial volume ratios $V_{melt} / V_{atm.} / V_{purge} \cdot h = 1 / 2 / 10$
- $T = 600\,°C$
- Purge: synthetic air




- Example case ($k_{Dec} = 6.0 \cdot 10^{-12}\,\frac{m^6}{s \cdot mol}$)




1. Measure evolution of nitrous gases at different temperatures.
2. Find simulation curves that fit the experimental data

→Confirmation of rate law and rate constants

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