Analysis of MOCKA experiments for MCCI with stratified oxide and metal melts and internal heat generation by enthalpy feeding using the MEDICIS code

I. Bakalov (GRS), C. Spengler (GRS)**,** J. Foit (KIT),

ERMSAR 2015, Marseille March 24 – 26, 2015

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Introduction

- Recent MOCKA experimental program for simulation of MCCI with a stratified pool configuration at KIT (Germany)
  - Conduction of a series of MOCKA experiments with a simulant oxide/metal melt in a stratified configuration and different concrete types
    - ✓ Simulation of a long-term MCCI process by internal melt heating using energy generated by thermite and zirconium oxidation reactions
    - ✓ Large part (75%) of heating power is deposited to the oxide melt

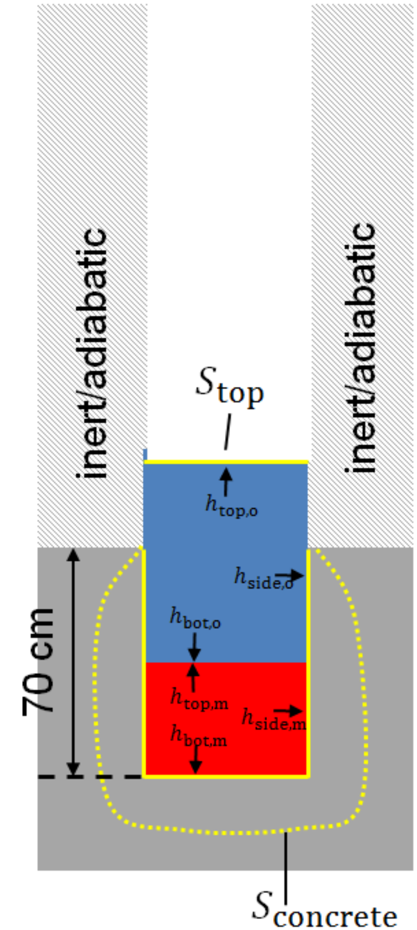
      ➡ prototypic heating of both melt phases (metal/oxide)
    - ✓ Investigation of erosion of concrete (incl. reinforced concrete) by both melt phases (metal/oxide), which was not possible in all former experiments (BETA, COMET-L, CCI etc.)
- GRS activities in the frame of MEDICIS validation program
  - Extension of MEDICIS validation work by analysing of selected MOCKA test series from the MOCKA experimental program at KIT (Germany)
    - ✓ MEDICIS analyses for two MOCKA test series (MOCKA 6 and MOCKA 3)
    - ✓ Special focus on simulation of internal melt heating by “enthalpy” injection to the melt, i.e. pouring of thermite and zirconium to the oxide phase

MOCKA experiments

- MOCKA experiments at KIT (Germany)
  - Cylindrical concrete crucible with an inner diameter 25 cm and height 70 cm
    - Cylindrical wall with z ≤ 70 cm LCS or siliceous concrete (with/without Fe rebars)
    - Cylindrical wall with z > 70 cm - inert material (ceramics)
      - No ablation during the experiment
- MOCKA 6.1 test series
  - Concrete crucible - LCS (without Fe rebars)
  - Initial melt composition:
    - Metal melt - 42 kg Fe and 4 kg Zr
    - Oxide melt - 68 kg oxides (initially Al_2O_3, CaO)
  - Internal melt heating simulated by using energy from chemical reactions of thermite (Fe_3O_4 + Al) and Zr
    - Total mass of 300 kg thermite and 104.4 kg zirconium supplied to the oxide phase in portions with time intervals
    - Thermite and Zr addition at ambient temperature 20 °C
    - Internal heating period - about 38.5 min (~ 2315 s)
  - Initial height of metal melt ~ 13 cm
  - Initial melt temperature ~ 1900 °C (~ 2173 K)

MEDICIS modellig approach

- MEDICIS parametric study
  - Study of basic aspects of MOCKA tests with MEDICIS
- MEDICIS modelling assumptions
  - Stratified melt configuration
    - ✓ Metal layer at the bottom, covered by oxide top layer
  - Concrete crucible – as a deep enough cavity
    - ✓ Lower crucible section z ≤ 70 cm – LCS concrete
    - ✓ Upper crucible section z > 70 cm – $T_{abl.}$ > 3000 K
    - ➡ to simulate refractory material
  - Simple assumptions
    - ✓ No material ejection at top melt surface
    - ✓ Consideration of radiation heat at top melt surface
    - ➡ no thermal losses to ceramic block (adiabatic)
    - ✓ Small heat losses at top interface - initial ratio: $S_{top}/S_{concrete} \approx \frac{1}{10}$
  - Empirical heat transfer coefficients - based on evaluations of previous 2D MCCI experiments (BETA, COMET etc.)
    - ✓ Oxide/concrete interface: $h_{bot,o}$: 500 W/(m²K), $h_{side,o}$: 300 W/(m²K)
    - ✓ Metal/concrete interface: $h_{bot,m}$: 500 W/(m²K), $h_{side,m}$: 1000 W/(m²K)
    - ✓ Top melt surface: $h_{top,o}$: 10 kW/(m²K)
    - ➡ to account for high average $T_{surface}$ evaluated in the experiment



Results of MEDICIS calculations

- Effect of modeling of “enthalpy” injection to the oxide layer

Background

- Simulation of internal heating requires a careful treatment of the boundary conditions representing the addition of thermite and Zr to the oxide melt

Method of analysis

- Comparative analysis of two modeling approaches for simulation of reactive material injection (Fe_3O_4+Al and Zr) to the upper oxide melt phase

Modellig approaches

- Continuous injection of thermite and zirconium to oxide melt
  - ✓ Constant material flow, determined on the bases of total material masses injected over the experimental time
  - ✓ Material injection without considering the time intervals for addition of reactive material
- Detailed injection of thermite and zirconium to oxide melt
  - ✓ Actual material flow as in MOCKA experiments (detailed injection tables)
  - ✓ Material injection in portions considering the time intervals for addition of each component according to the experimental time sequence

Results of MEDICIS calculations

- Effect of modeling of “enthalpy” injection to the oxide layer

Continuous injection:

Higher erosion power to concrete

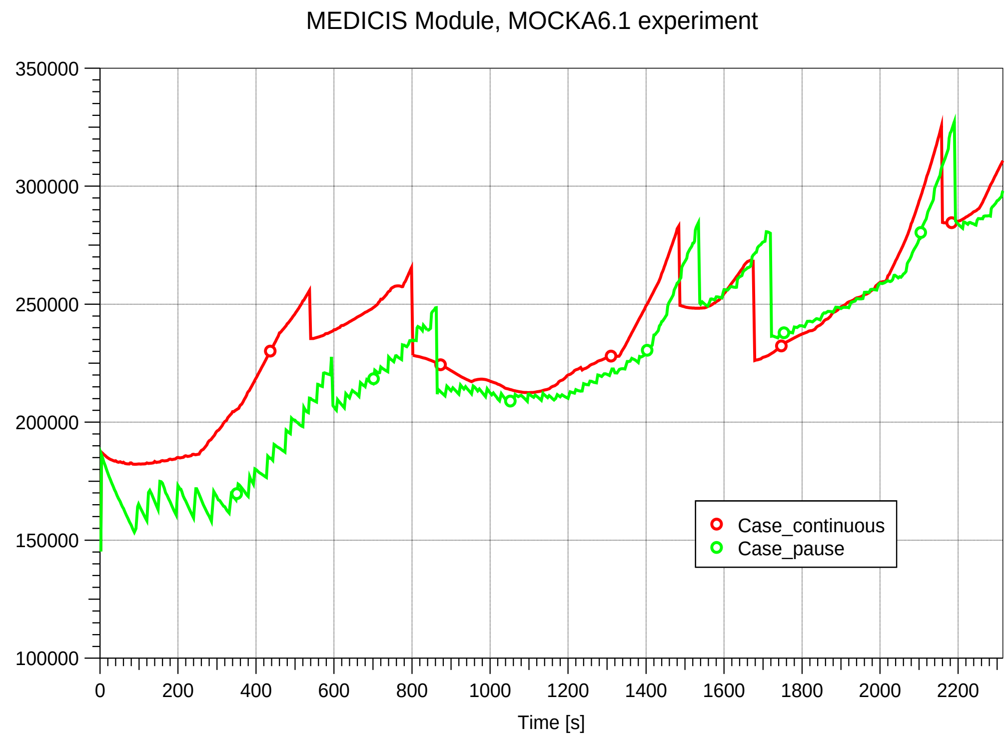
➡ larger concrete erosion depth

- Injection of material starts at t = 0 s

Detailed injection:

Lower erosion power to concrete

- Actual injection of material starts at t = 92 s



In both cases, the erosion power shows a constant tendency to increase over the time

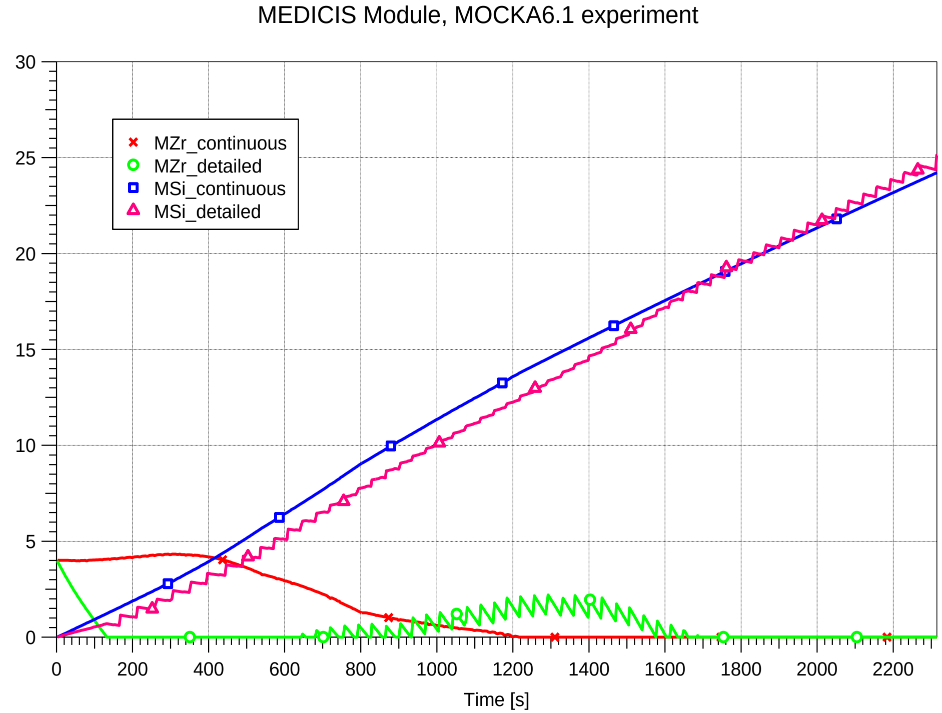
- No quasi-steady state is reached within the experimental time:

  Gas release rate is not enough to provide oxygen for completing the chemical reactions in the melt

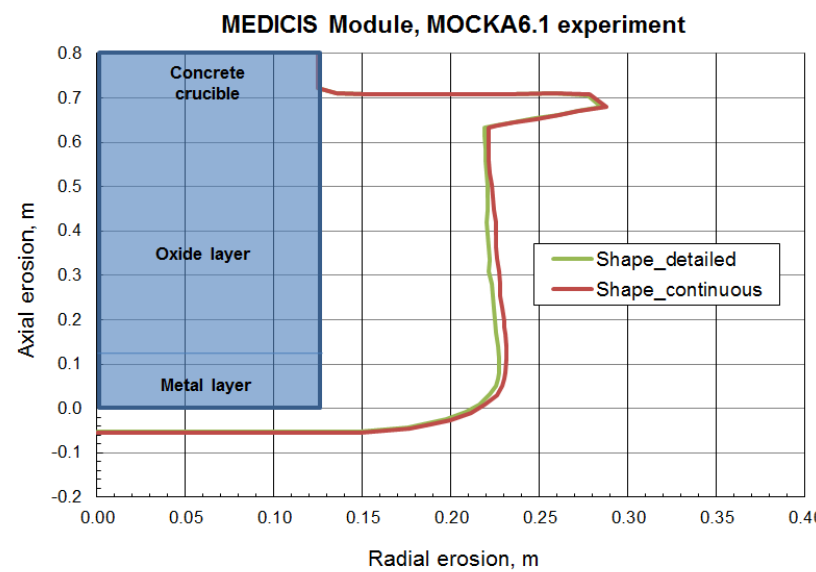
  Temperature gradient/HTC are not enough to transfer all the internal power to the concrete walls

Results of MEDICIS calculations

- Effect of modeling of “enthalpy” injection to the oxide layer



Parameters	Experiment	MEDICIS (Continuous)	MEDICIS (Detailed)
$h_{bot.}/h_{side}$, (W/m2*K)	-	500/1000	500/1000
Erosion volume by metal layer, (l)	~ 17….18	39	36
Erosion volume by oxide layer, (l)	~ 84	52	50
Total erosion volume, (l)	~ 101…102	91	87



Detailed injection:

Full oxidation of Zr mass, initially present in the melt

as originally planned by the KIT experts

More realistic simulation of “enthalpy” injection to the oxide melt

Internal power release and subsequent erosion rate depend on the presence of oxygen, which is provided through concrete erosion

Results of MEDICIS calculations

- Effect of slowed-down mass transfer of species between the oxide and metal melt layers

<u>Background</u>

- MEDICIS validation results showed a tendency for:
  - underestimation of energy released in oxide layer (underestimation of concrete erosion by oxide layer)
  - overestimation of energy released in metal layer (overestimation of concrete erosion by metal layer)

<u>Supposed reason</u>

- Fast mass transfer between the melt layers when distributing the particular melt species between the oxide/metal phases

→ Investigation of the effect of mass transfer between melt layers on the ablation depth by slowing down the mass transport of species from oxide to metal phase

<u>Investigated cases</u>

- Base case – very fast (instantaneous) mass transfer from oxide to metal layer, as originally modeled in MEDICIS
- Sensitivity case – slowed-down mass transfer from top oxide to bottom metal layer using a time constant of τ = 100 s in MEDICIS

Results of MEDICIS calculations

- Effect of slowed-down mass transfer of species between the oxide and metal melt layers

Base case:

Zr mass added to the oxide layer is not fully oxidized during the experiment:

- Fast Zr mass transfer from the oxide to the metal phase
- Less energy transfer to the oxide layer

→ reduced local concrete ablation

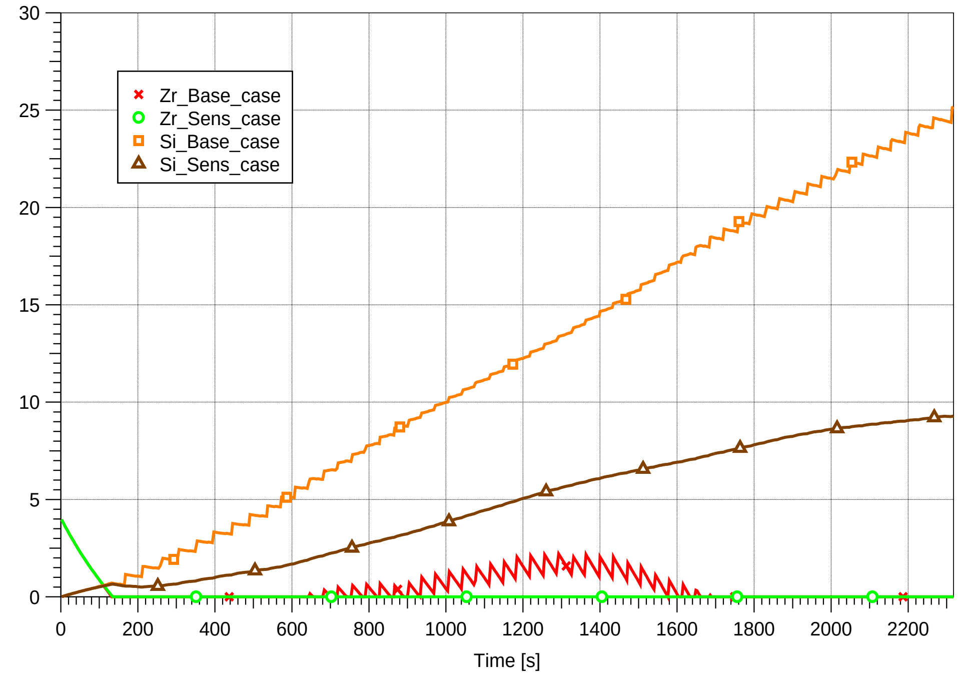
Sensitivity case:

- Full Zr oxidation by the gases from the concrete decomposition

→ Zr mass stays longer in the oxide layer

- Higher energy transfer to the oxide layer

MEDICIS Module, MOCKA6.1 experiment



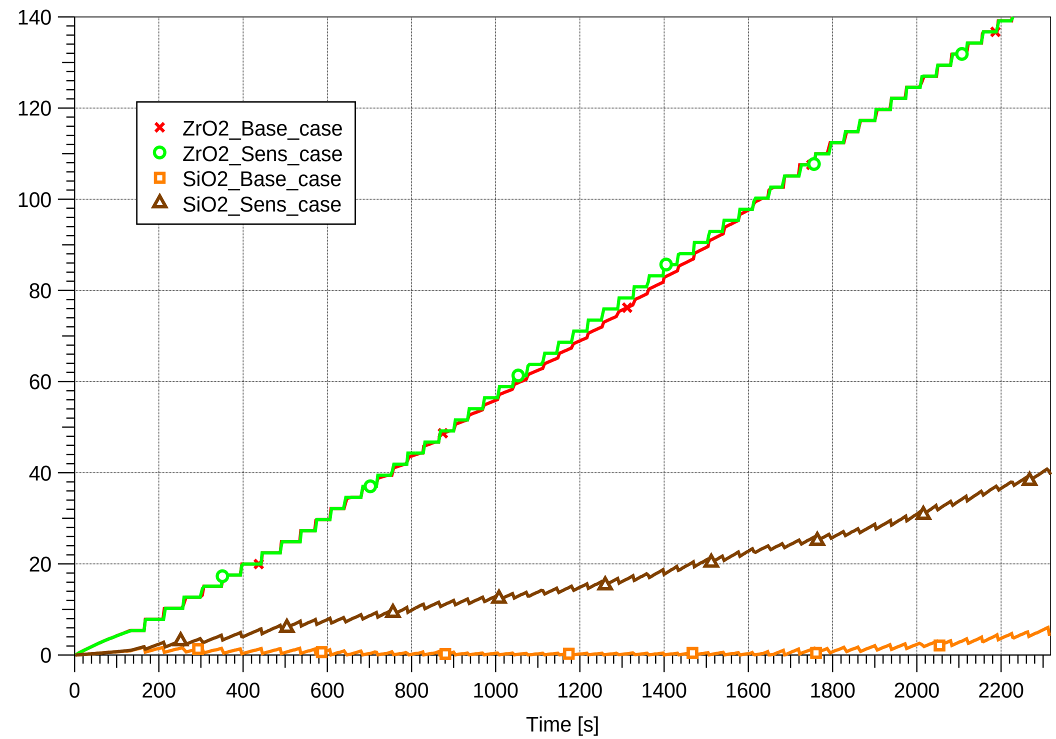
Sensitivity case shows a significantly smaller amount of Si in the metal phase

- More Si mass is oxidized by the gases (H_2O and CO_2) → accumulation of SiO_2 in the melt

Results of MEDICIS calculations

- Effect of slowed-down mass transfer of species between the oxide and metal melt layers

MEDICIS Module, MOCKA6.1 experiment



Sensitivity case leads to accumulation of larger amount of SiO_2 in the oxide phase

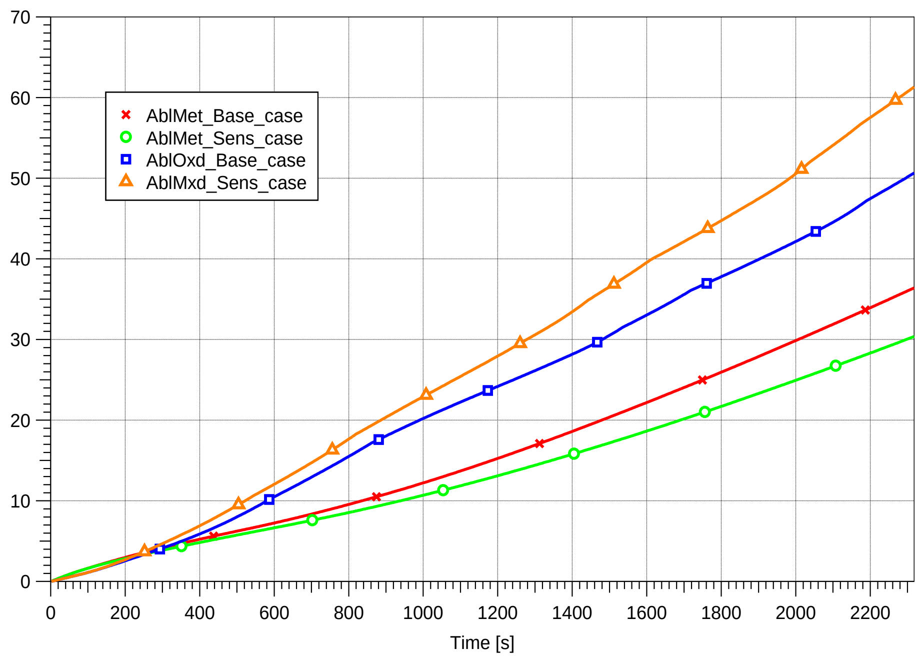
- Higher Si oxidation by the gases from the concrete decomposition

➡ higher energy release to the oxide phase

Results of MEDICIS calculations

- Effect of slowed-down mass transfer of species between the oxide and metal melt layers

MEDICIS Module, MOCKA6.1 experiment



Parameters	Experiment	MEDICIS (Base case)	MEDICIS (Sens. case)
$h_{bot.}/h_{side}$, (W/m2*K)	-	500/1000	500/1000
Erosion volume by metal layer, (l)	~ 17….18	36	30
Erosion volume by oxide layer, (l)	~ 84	50	62
Total erosion volume, (l)	~ 101...102	87	92
Sidewall ablation by oxide layer, (cm)	~ 12…15	9.9	10.2
Sidewall ablation by metal layer, (cm)	~ 9…12	10.1	10.4
Axial ablation by metal layer, (cm)	~ 4	5.2	5.3

Sensitivity case results in:

- Larger erosion volume by the oxide layer
  → higher energy release in the oxide phase resulting from higher Zr and Si oxidation
- Smaller erosion volume by the metal layer → lower energy release

<u>Sensitivity case results show a better agreement with the experimental data</u>

Conclusions

- **<u>MEDICIS results for MOCKA test series have a transient character</u>**
  - Erosion power to the concrete increases over the time, while injecting a constant mass of reactive material into the melt (enthalpy feeding)
- MEDICIS calculations do not reach a quasi-steady state within the experimental time
  - Required gas release rates or temperature gradients at assumed heat transfer coefficients are not reached
- A detailed modeling of the reactive material addition gives a more realistic simulation of “enthalpy” injection to the oxide melt
  - Consideration of actual mass increments and time intervals for adding the material components to the melt
- Strong influence of the mass transfer between the melt layers on the internal power distribution within the melt
  - Original MEDICIS model assumes a rather fast (instantaneous) mass transfer of species between the melt layers
  - A model with slow mass transfer from the upper to lower melt layer might be reasonable to be tested

Conclusions

- **Consideration of a more realistic case with higher heat losses at the top melt surface as in real MOCKA test series**
  - Larger melt surface area due to the conical construction at the top of the concrete crucible
- **Evaluation of the MEDICIS results for MOCKA test series underlines the following points:**
  - Difficulty in providing a realistic simulation of the internal heat (decay heat) of the melt and in reducing the relevant uncertainties
  - Complexity of modelling of the MCCI issue

- **Outlook**
  - Measurements of the melt temperature in new MOCKA experiments could provide more insights
    - ✓ Indication for correct estimation of the heat transfer distribution
  - Investigation of the impact of iron rebar (concrete reinforcement) on the concrete ablation
    - ✓ Important for transposition from experiments to reactor case

Acknowledgements

- The work presented in this paper is subject of R&D-projects financed by the German Federal Ministry for Economics Affairs and Energy (BMWi) under the contract numbers RS1508 and of the EU-CESAM project.

Thanks for your attention!