

# GTT User meeting – 2022

## Application of private database development feature in FactSage for modeling the liquid steel solution

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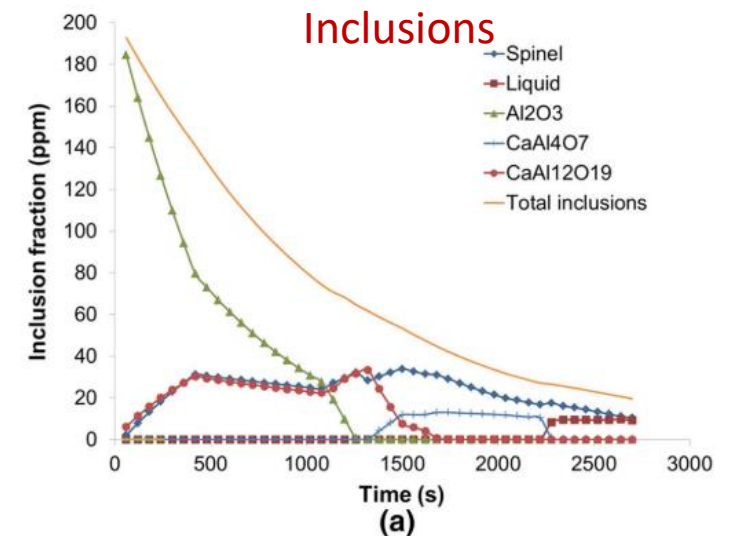
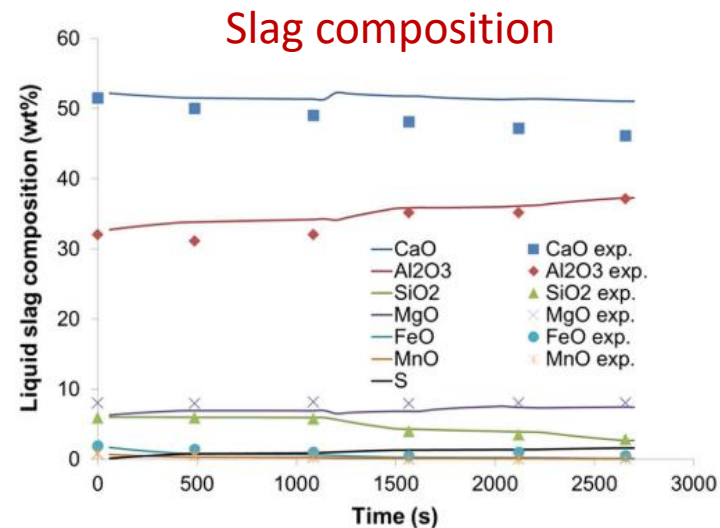
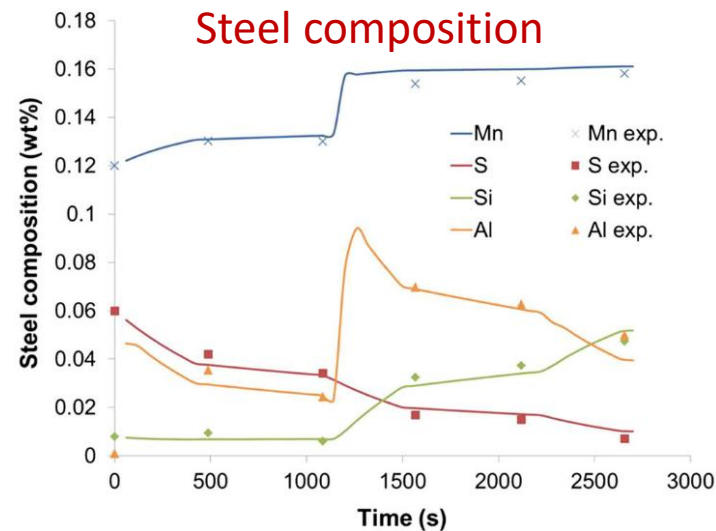
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- Issue of calcium solubility
- Development of a private database in FactSage
- Comparison with FTmisc (Fe-Ca-Al-Mg-O system)
- Predicted calcium pick-up: steel-slag reaction
- Conclusions

# Introduction

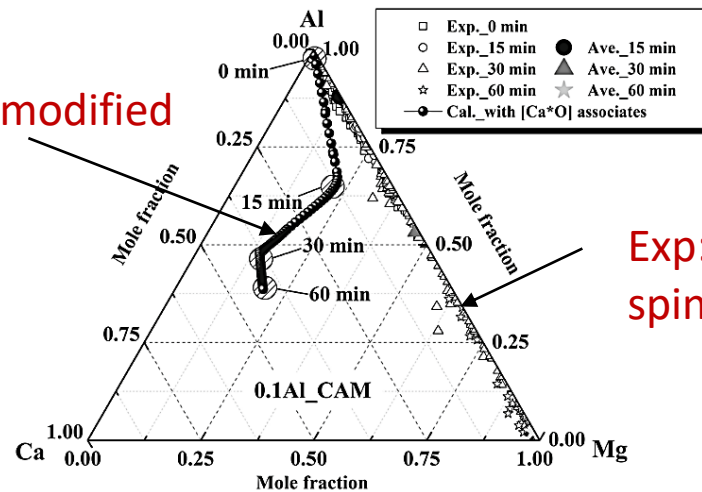
- Steelmaking process: BF-BOF/EAF → **Ladle/RH/VD** → continuous casting
- Secondary steelmaking: composition adjustment, clean steel
- Modeling work:
  - Earlier focus: mixing in ladle, composition change of steel and slag
  - Recent focus: comprehensive model to determine changes in steel, slag and inclusion during secondary steelmaking; FactSage is popular here



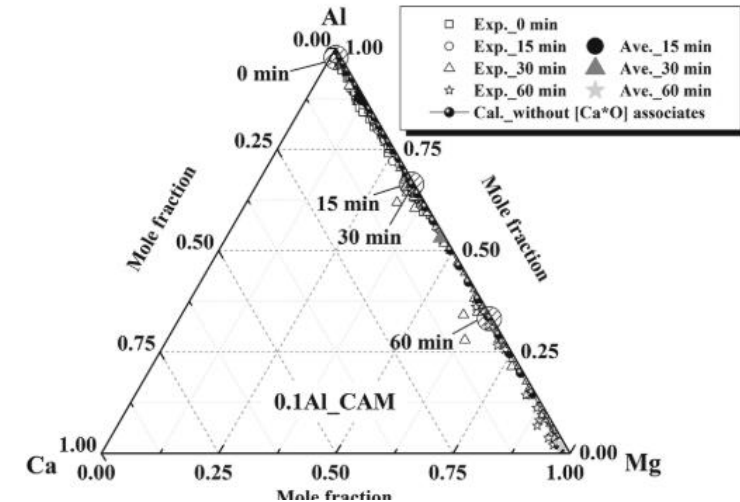
# Inclusion prediction models

- Reaction between Al-killed steel and CaO, MgO saturated slag
- FactSage based kinetic model tends to predict higher CaO content in inclusions
- FT-misc without Ca\*O associate shows better agreement with exp. for 0.1% Al
  - But it does not explain Ca pick-up in inclusions for other cases

Model: fully modified inclusion



Exp: Al<sub>2</sub>O<sub>3</sub> → spinel → MgO



Steel (0.1% Al) with CAM slag in MgO crucible

Model: FTmisc with associate

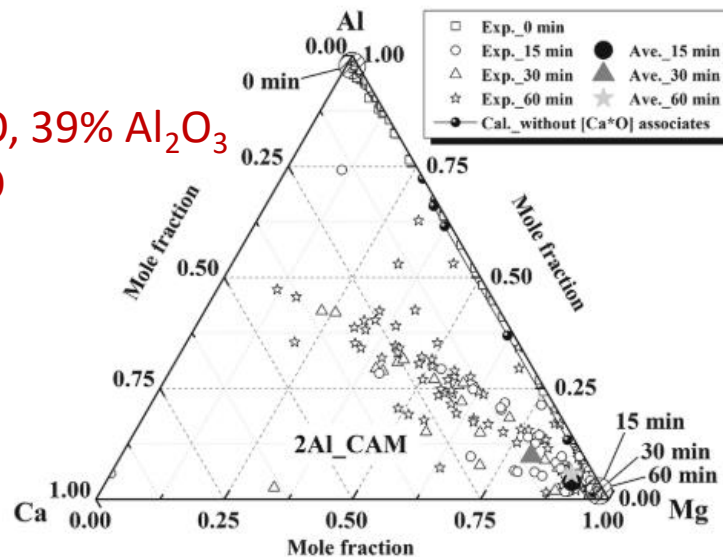
Steel (0.1% Al) with CAM slag in MgO crucible

Model: FTmisc without associate

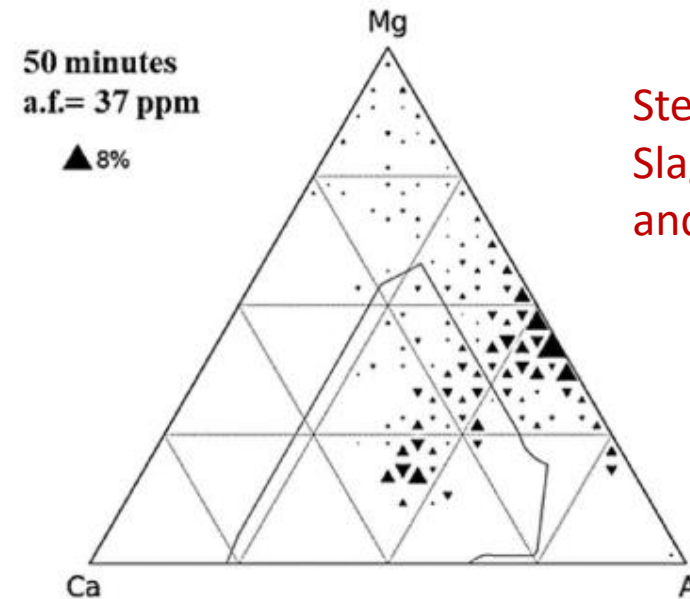
# Conditions for calcium pick-up

- Combinations of slag composition, crucible material were tested
- Conditions for significant calcium pick-up in inclusions (without calcium treatment):
  - 2% Al containing steel in contact with double saturated slag
  - Addition of 1% electronic grade silicon in Al-killed steel in contact with double saturated slag
- Ignoring  $\text{Ca}^*\text{O}$  associate does not help here!

Steel: 2% Al  
Slag: 51% CaO, 39%  $\text{Al}_2\text{O}_3$   
and 10% MgO



Ref: Liu et al., MMTB, 51B (2020), 529-542



Steel: 0.3% Al  
Slag: 51% CaO, 42%  $\text{Al}_2\text{O}_3$   
and 7% MgO

Ref.: Kumar & Pistorius, MMTB 52B(2021), 163-177

# Current approach

- Create an associate solution for liquid Fe using solution module in FactSage (private database)
- The free energy of associate formation for  $\text{Al}^*\text{O}$ ,  $\text{Al}^*\text{O}^*\text{Al}$  and  $\text{Mg}^*\text{O}$  are found to match FTmisc
- Adjust free energy of formation for  $\text{Ca}^*\text{O}$  that can explain experimental observations

FactSage 8.1: Solution

File Edit Units Options Tools Help

Function Name  FeAlsoln.Func(CaO#FeLQ\_0032A)

Function Name  FeLQ\_0032A

$\Delta H_{298} \text{ J/mol}$	$S_{298} \text{ J/(mol K)}$
-100000	-29.100784828

TMin (K)  298.15 TMax (K)  2500  1/1

Cp(T) J/(mol K)  0

Thermal expansivity (/ K)

Compressibility (/ bar)

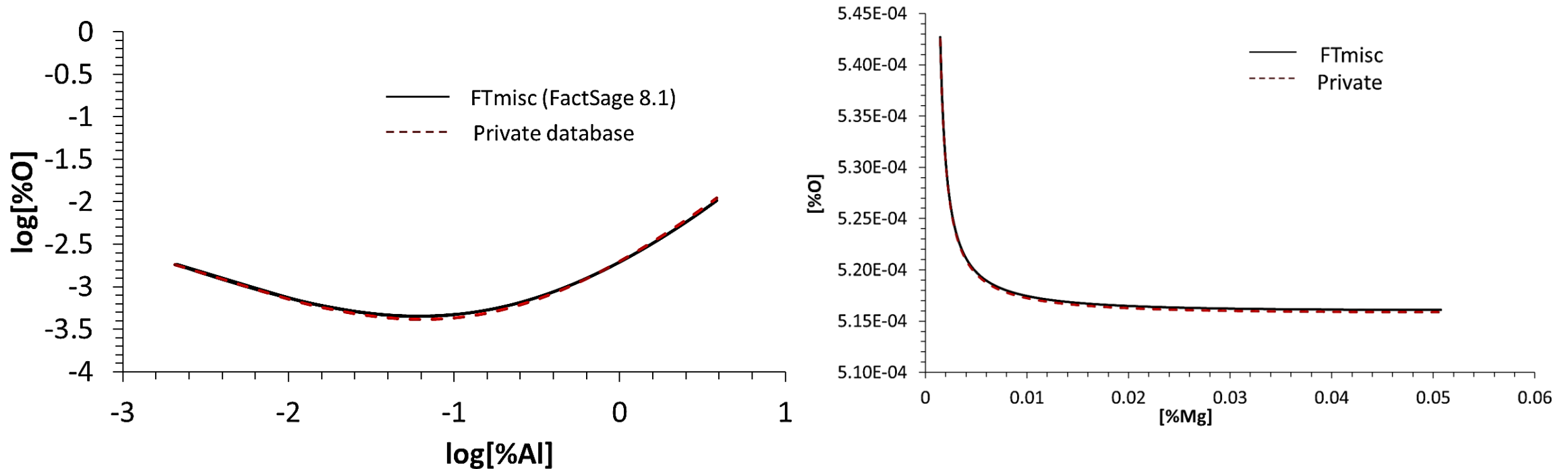
Bulk modulus derivative

FeAlsoln

- Functions
  - O (1)
  - Mg (1)
    - FeLQ\_0060 (1)
  - MgO (2)
    - FeLQ\_0061 (1)
    - FeLQ\_0061A (1)
  - Al (1)
  - AlO (2)
  - Al2O (2)
  - S (1)
  - Ca (1)
  - CaO (2)
    - FeLQ\_0032 (1)
    - FeLQ\_0032A (1)**
  - Fe (1)
- Solutions (1)
  - FeLQ (2-1) (WAGN)
    - SubLattice
    - End Members (10)
    - Mixables (0)
    - Interactions (21)
      - (0) AL
      - (1) AL:AL
      - (2) AL:CA
      - (3) AL:O
      - (4) CA
      - (5) CA:CA
      - (6) O
      - (7) O:O
      - (8) Ca\*O
      - (9) AL:AL:AL
      - (10) Al -Al\*O

# Fe-Al-O and Fe-Mg-O: FTmisc vs Private

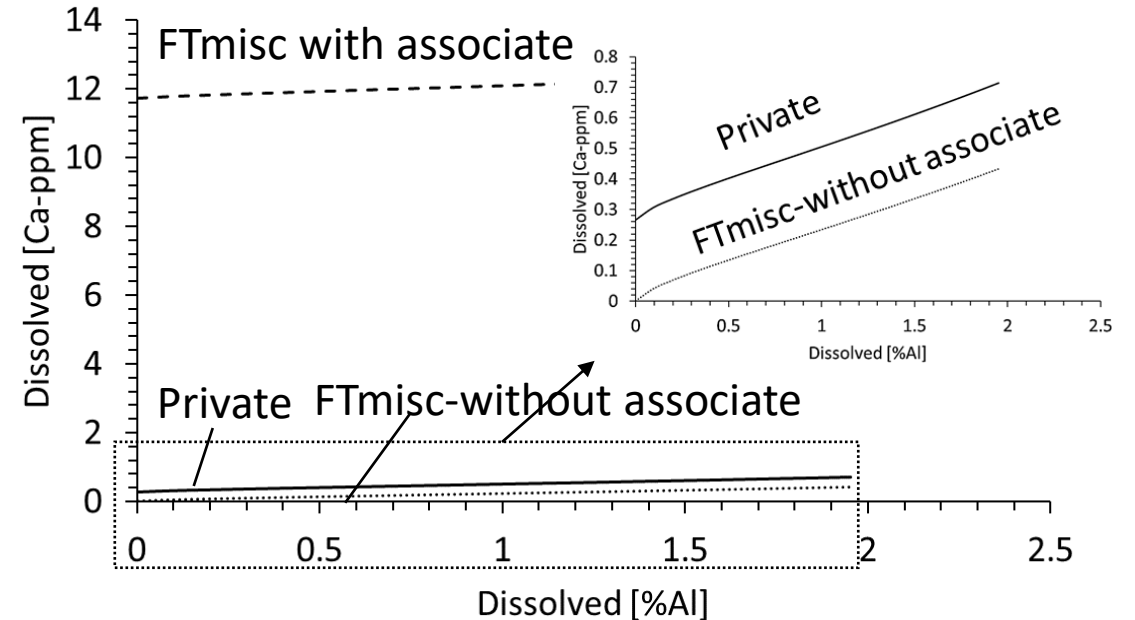
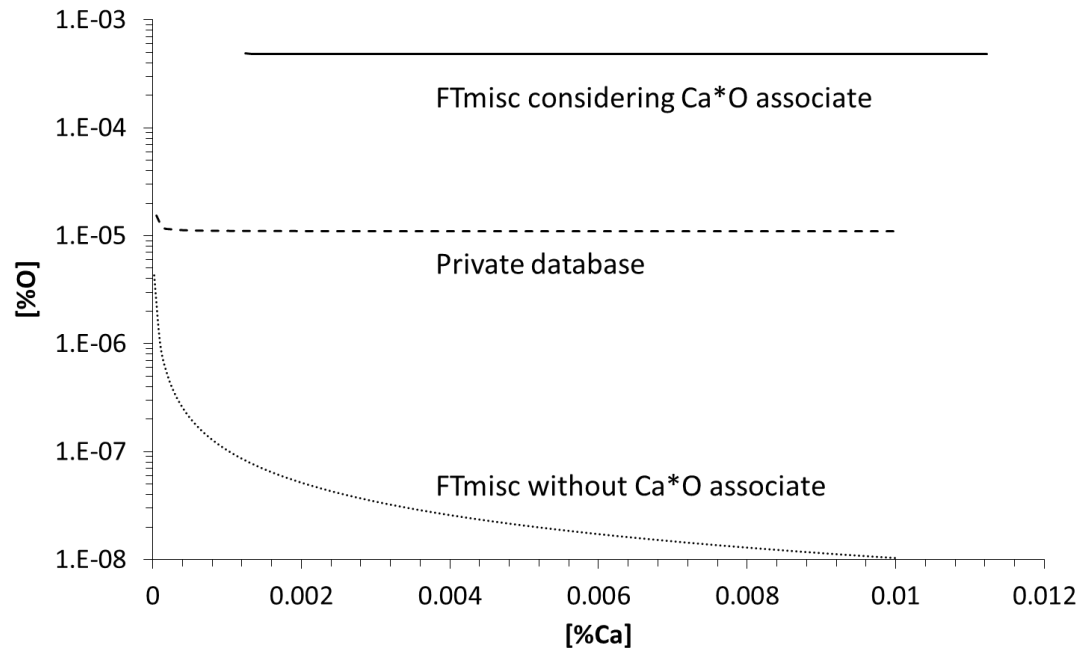
- The agreement between FTmisc and the private database is good for Fe-Al-O and Fe-Mg-O system



# Calcium solubility: FTmisc vs private database

- Private database considers limited Ca\*O associate formation
- $a_{\text{CaO}} = 1$

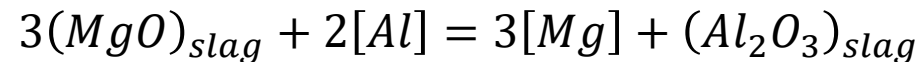
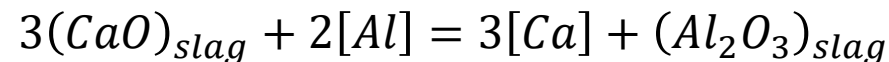
- 500 g of steel containing variable amount of Al is equilibrated with 75 g of slag (51% CaO, 39%  $\text{Al}_2\text{O}_3$  and 10% MgO)



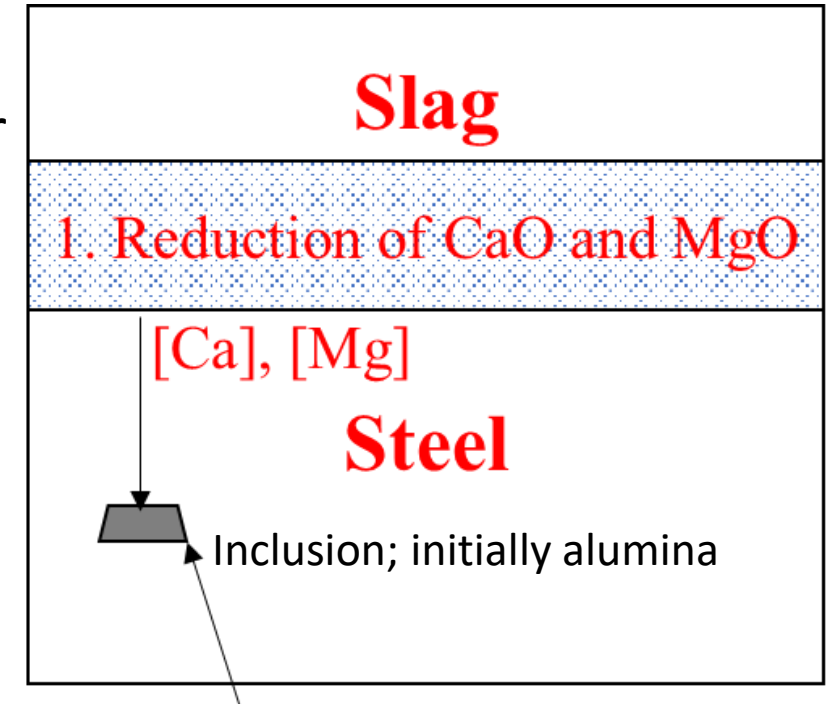


# Kinetic model

- Calcium solubility is too low; difficult to measure
- Measuring inclusion composition is relatively easier
- Effective equilibrium reaction zone model
- Reactions/phenomena:
  - Steel-slag reaction
  - Steel-inclusion reaction
  - Inclusion flotation
- Inclusion transformation is a two-step process:
  - Reduction of CaO and MgO at the steel-slag interface

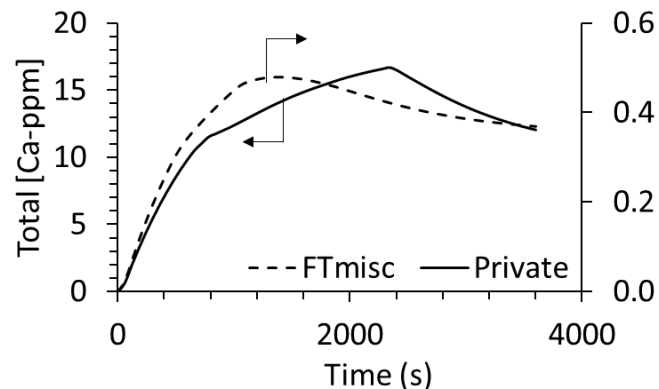
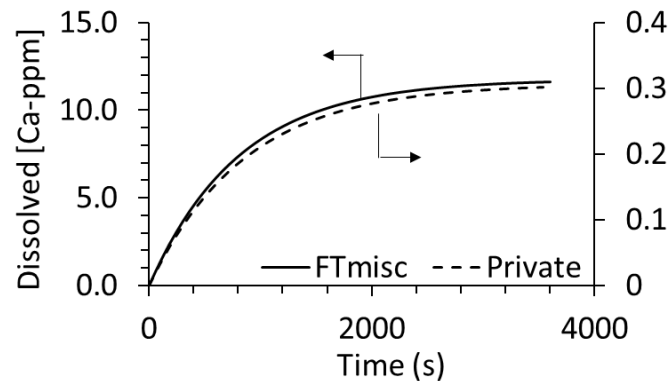


- Reduction of  $\text{Al}_2\text{O}_3$  at the steel-inclusion interface

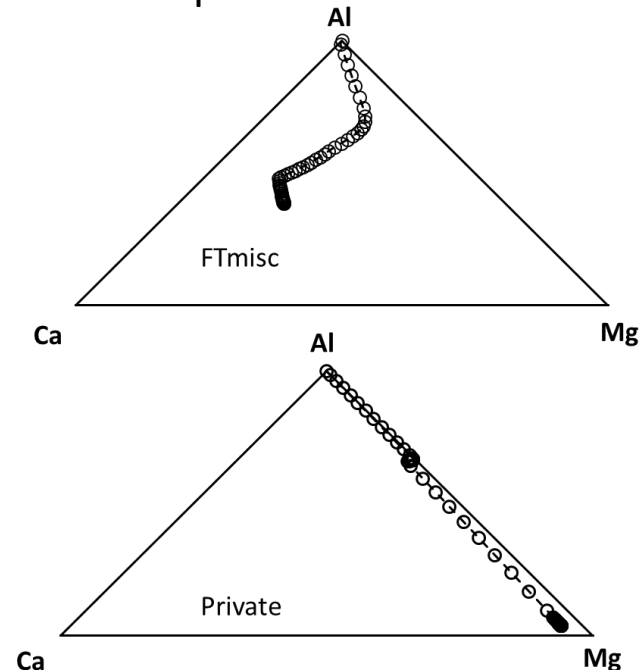


# Calcium pick-up: 0.1 wt% Al

- Dissolved calcium is about 50-times less for private database
- Decrease in total calcium is due to inclusion flotation
- Predicted inclusion composition from private database is closer to experimental observation

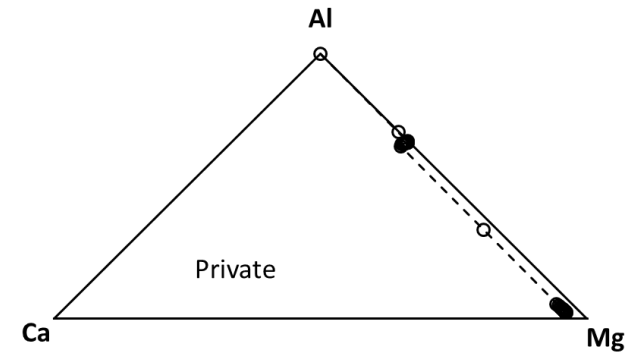
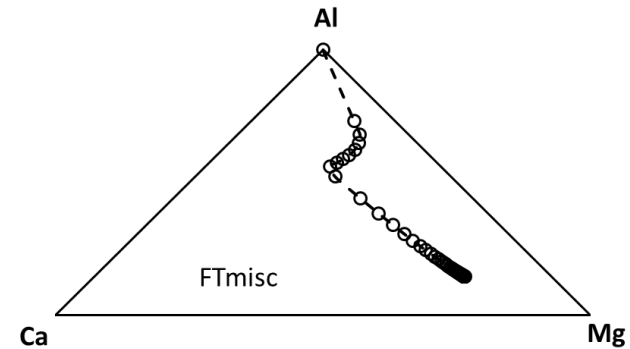
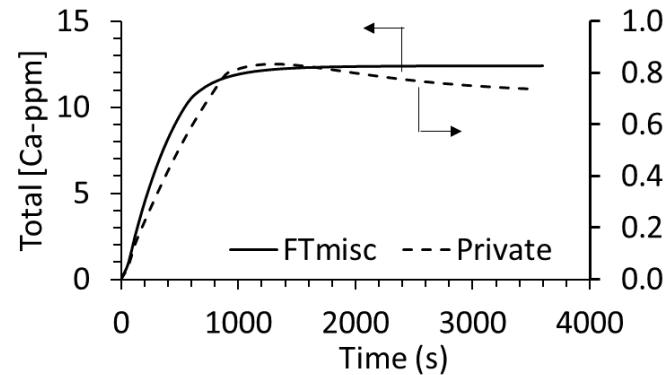
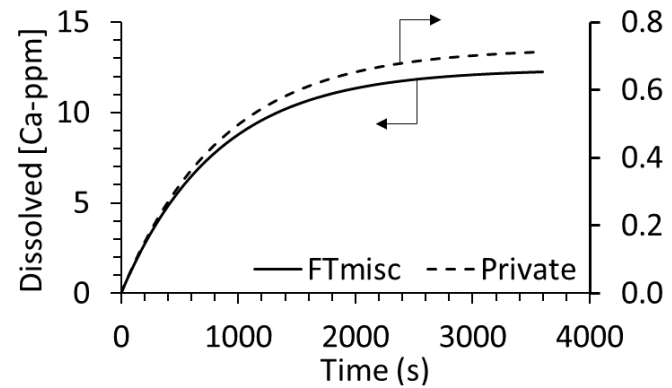


Inclusion composition: cation mole fraction



# Calcium pick-up: 2 wt% Al with slag

- Private database significantly reduces calcium pick-up by the melt
- Kinetics of Ca and Mg pick-up is much faster



# Conclusion

- An associate solution model developed in FactSage is an excellent tool to test experimental data
- Kinetic changes in inclusions during steelmaking may be used to test and understand the behavior of liquid steel solution
- More experimental data are required to resolve Fe-Ca-Al-Mg-Si-O system; silicon is to be incorporated

# Acknowledgment

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- Industrial Research and Consultancy Centre, IIT Bombay
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Thank you 😊  
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