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Efficient Storage and Recall of Slag Thermochemical Properties for Multiphysics Modelling

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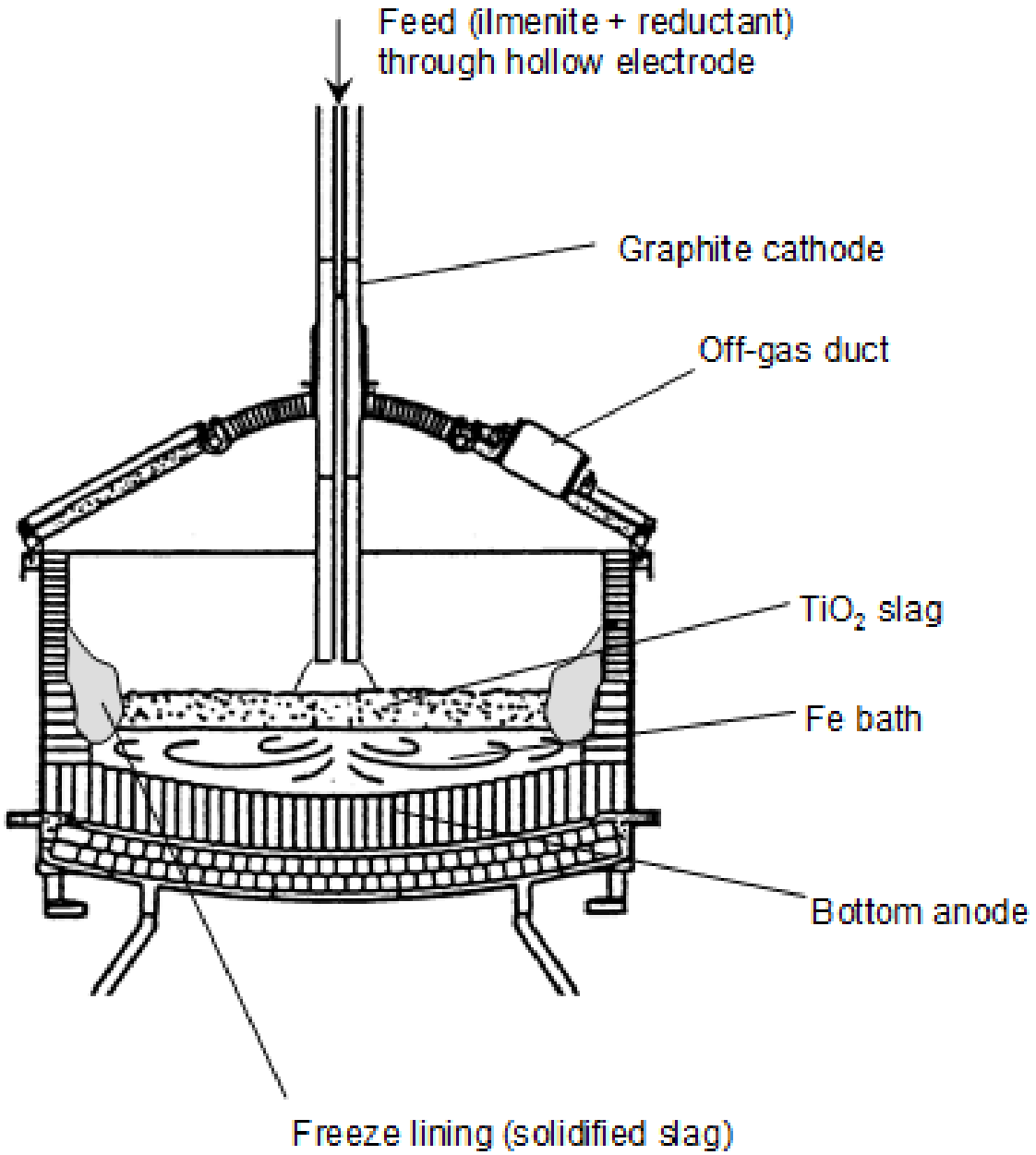
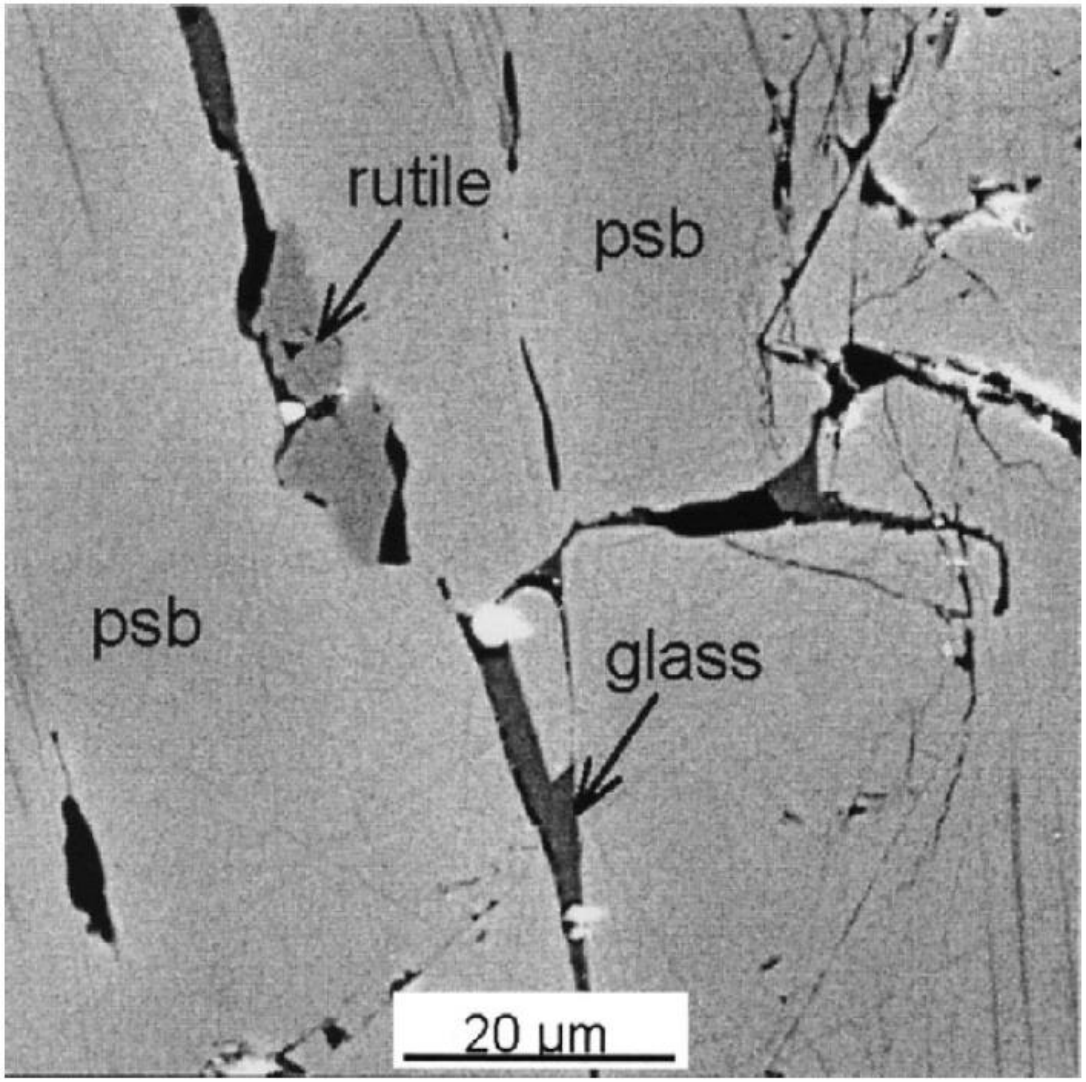
Background

Ilmenite Smelting

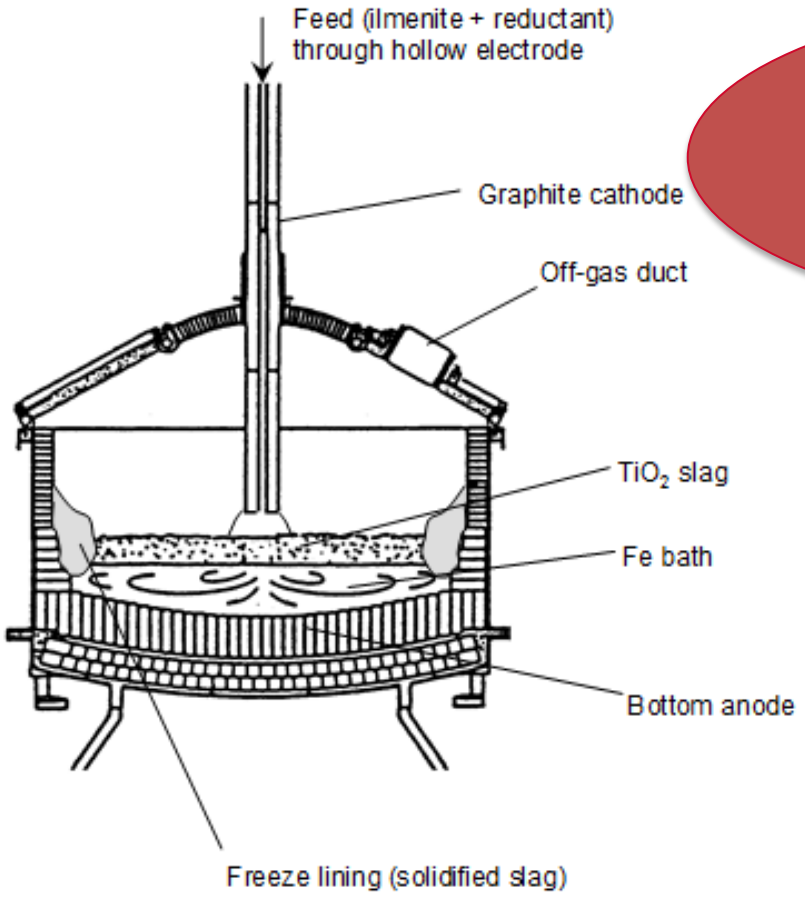


High-titania Slag
Predominantly Single Phase



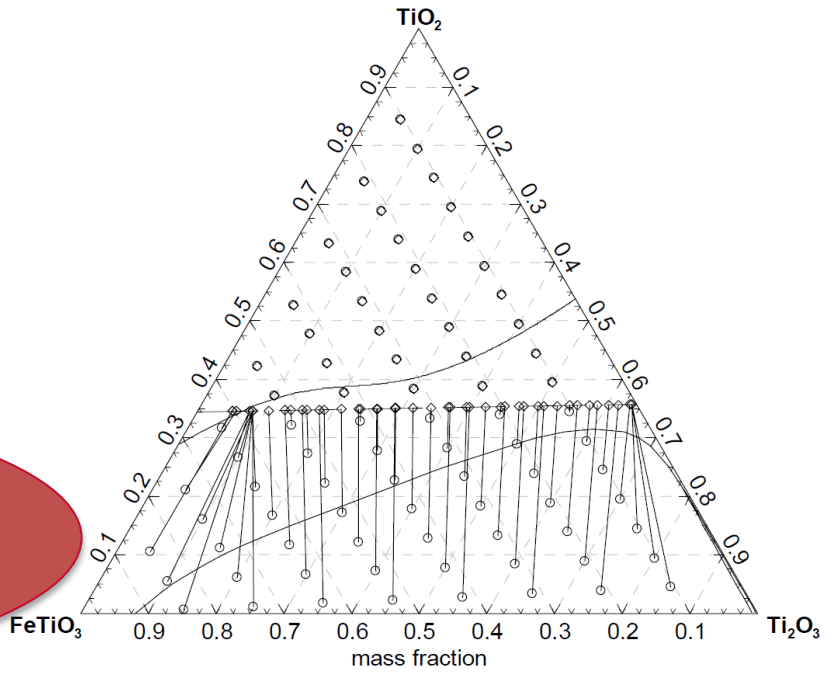
(Pistorius and Coetsee, 2003)

Combination of Factors



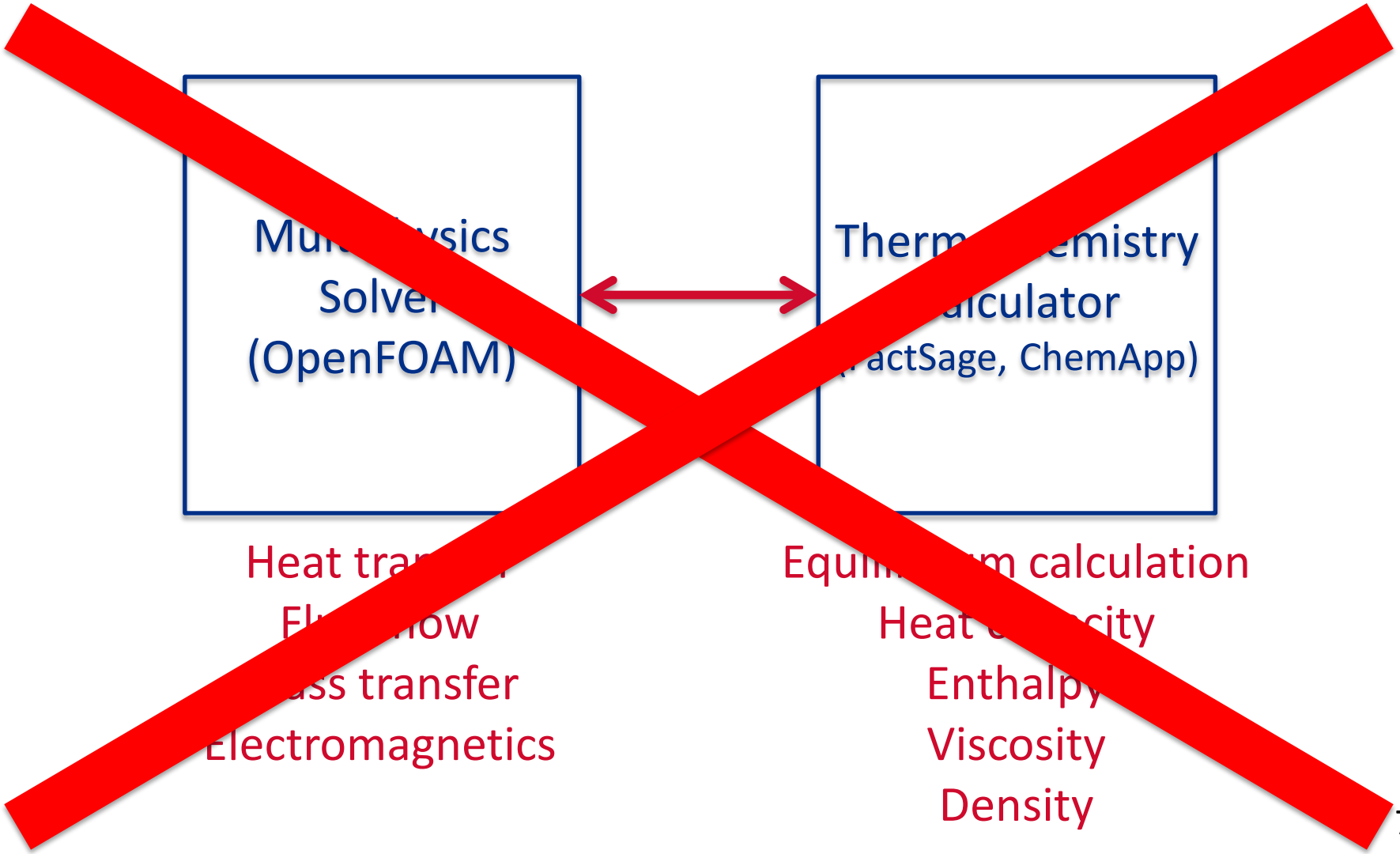
Heat Transfer
Fluid Flow

Thermochemistry

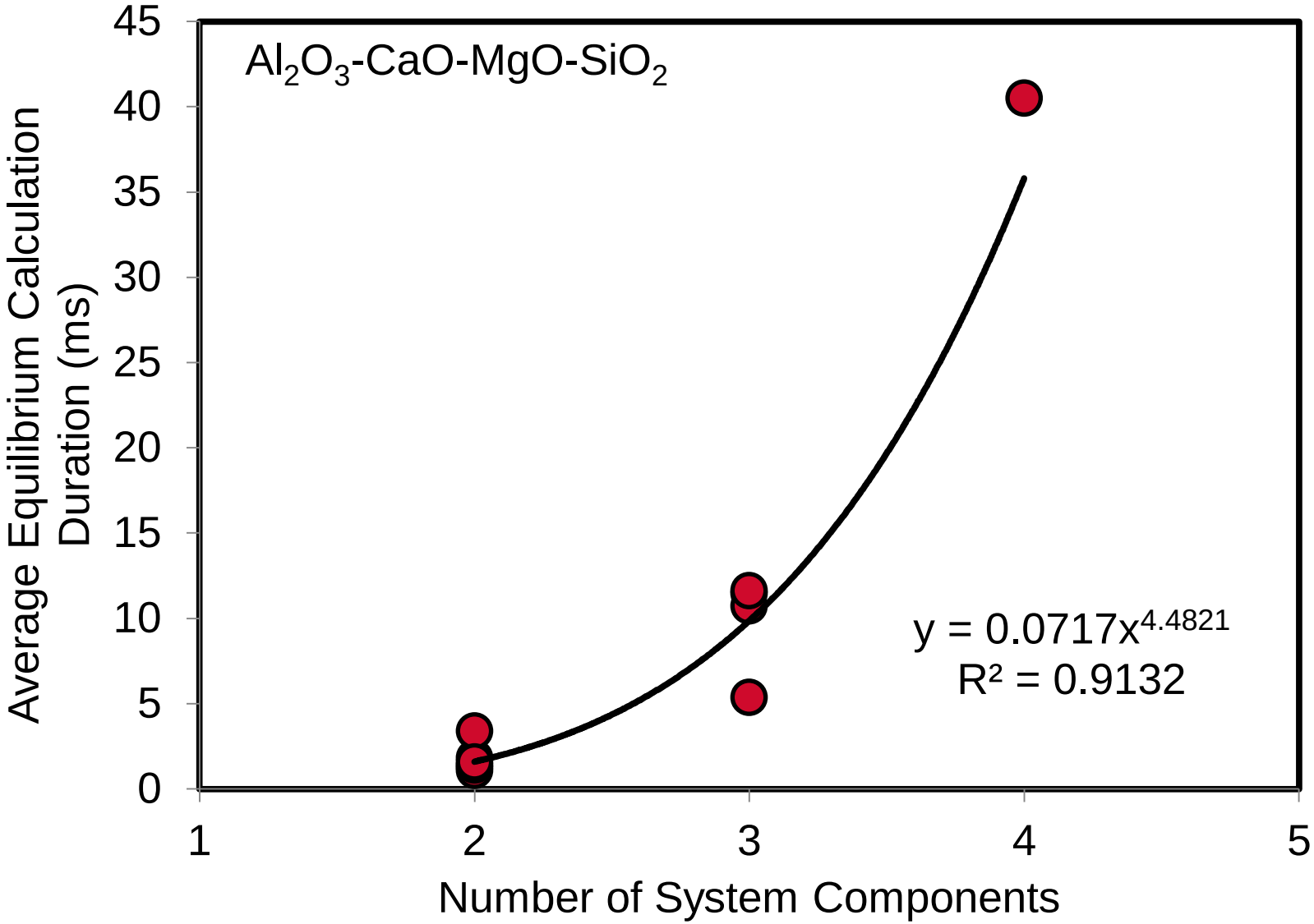


Concepts

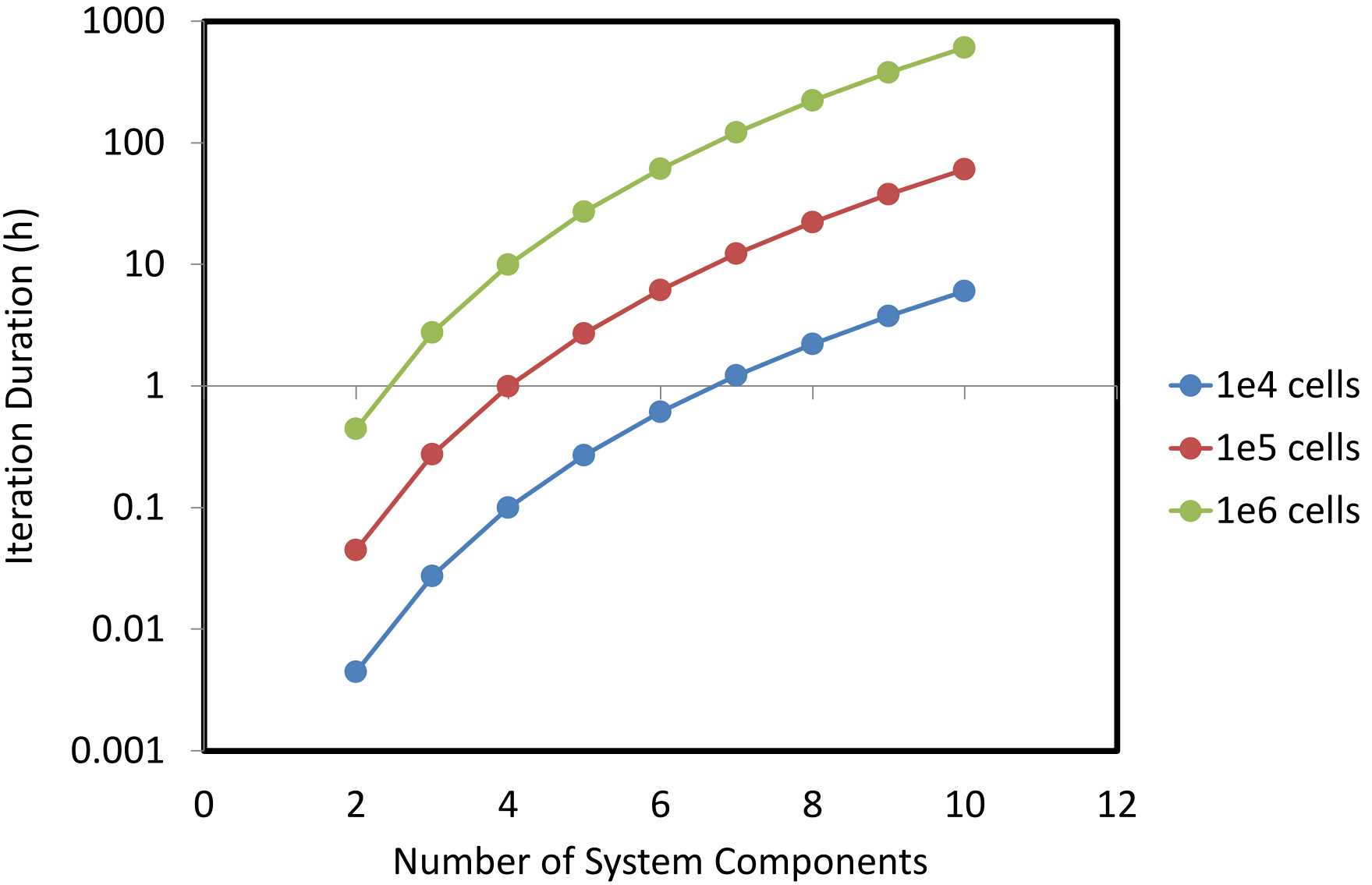
Comprehensively Describing Pyrometallurgical Processes



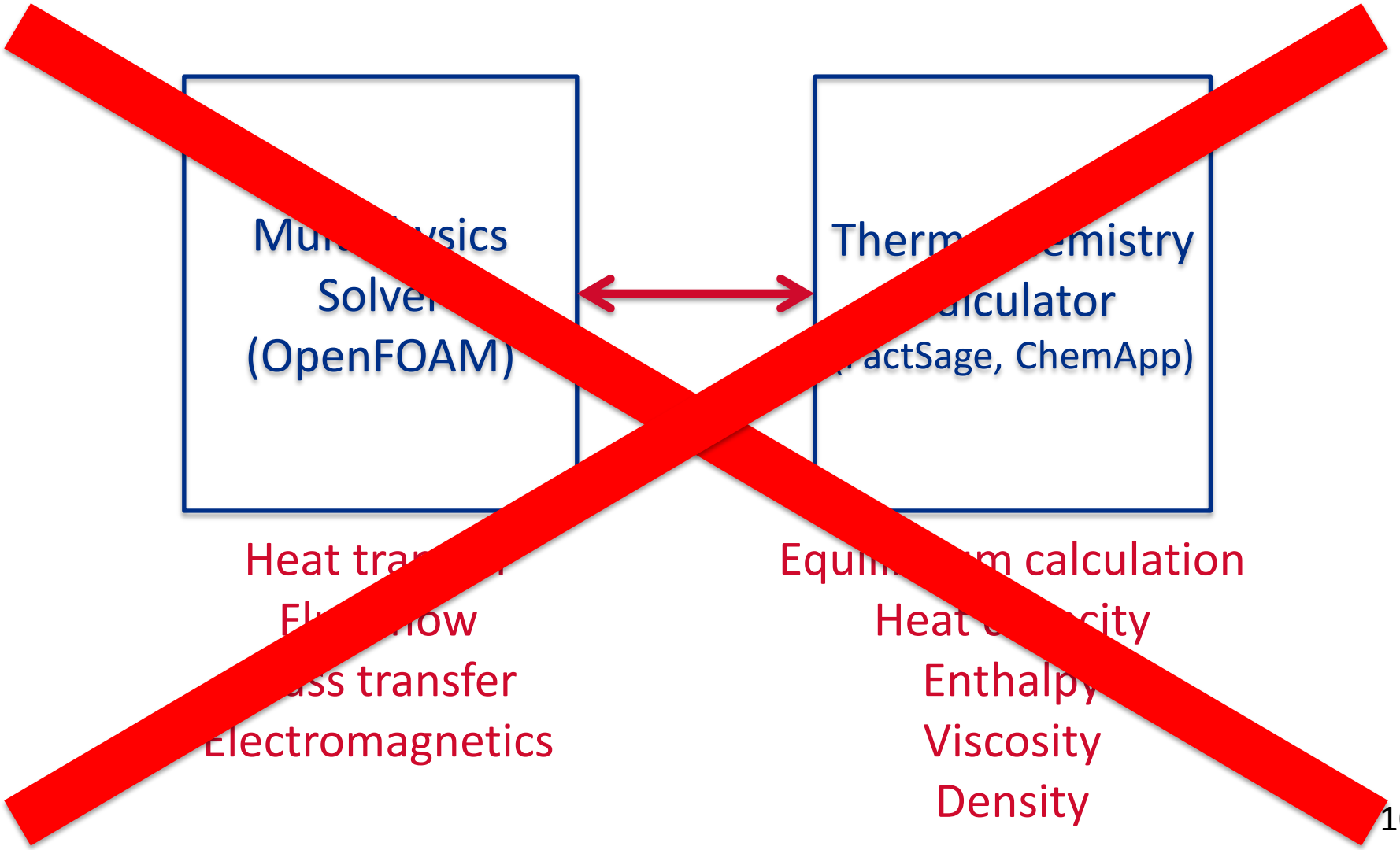
Computational Cost



Computational Cost



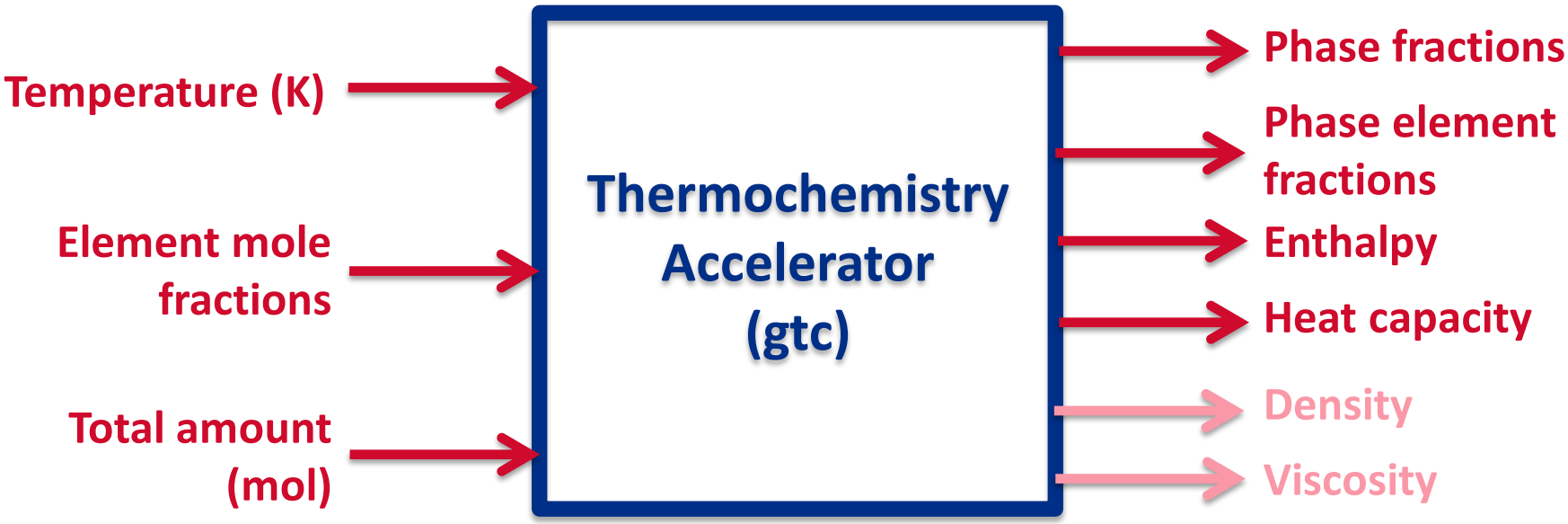
Comprehensively Describing Pyrometallurgical Processes



Comprehensively Describing Pyrometallurgical Processes

Heat transfer
Fluid flow
Mass transfer
Electromagnetics

Equilibrium calculation
Heat capacity
Enthalpy
Viscosity
Density


Temperature (K)
Element mole fractions
Total amount (mol)
Thermochemistry Accelerator (gtc)
Phase fractions
Phase element fractions
Enthalpy
Heat capacity
Density
Viscosity

Previous Work

Previous Work

- Not a new problem
- Aluminium casting examples
- Up to 4 system components
- Geometric approaches
- Limited use of thermochemistry theory
- No application to extractive metallurgy

Method

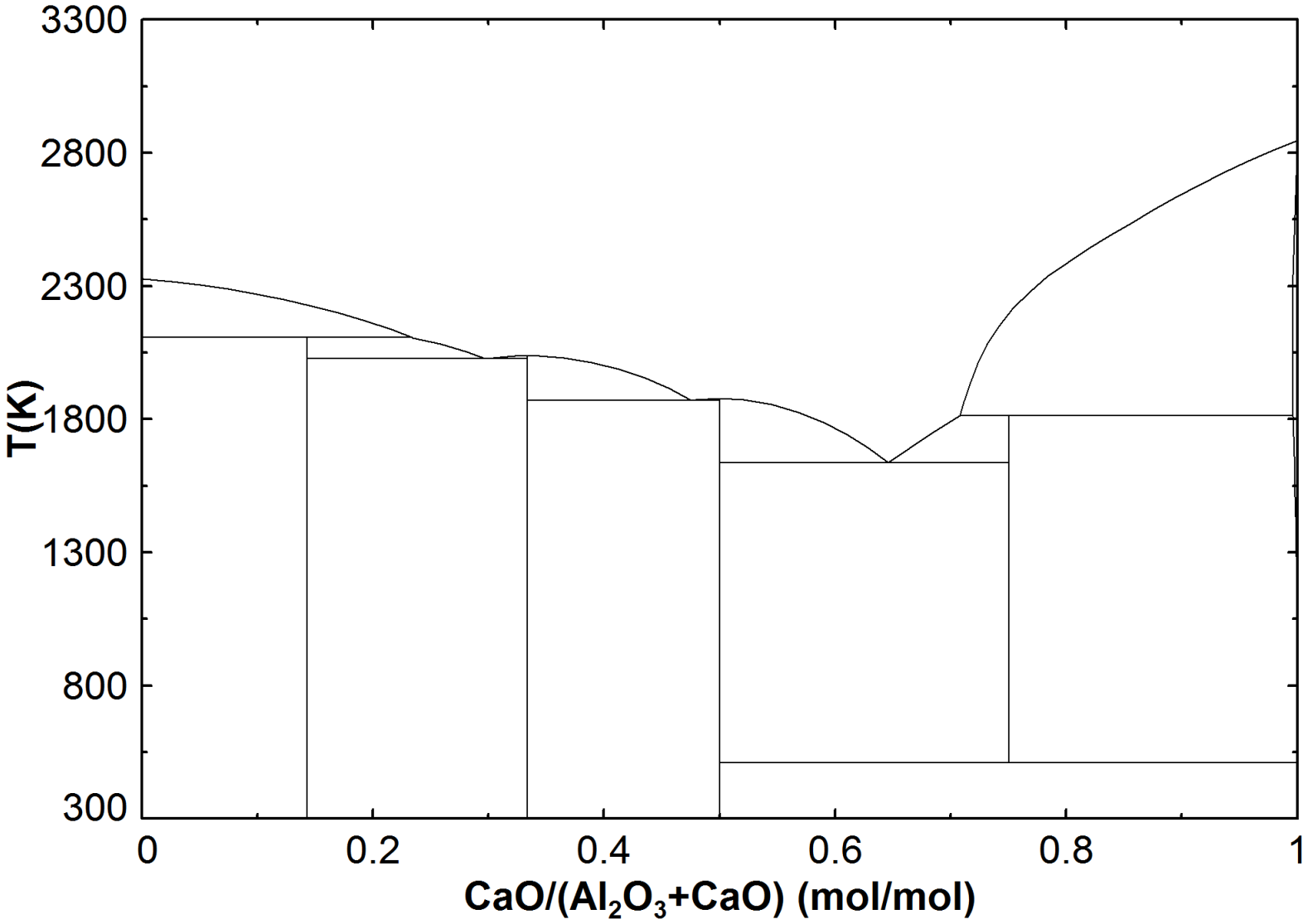
Decisions

- Start with binary and ternary systems
- Use a geometric approach
- Apply thermochemistry theory to
  - simplify and accelerate calculations;
  - minimise dimensionality of geometries; and
  - minimise storage and memory requirements.
- Implement prototype in Python

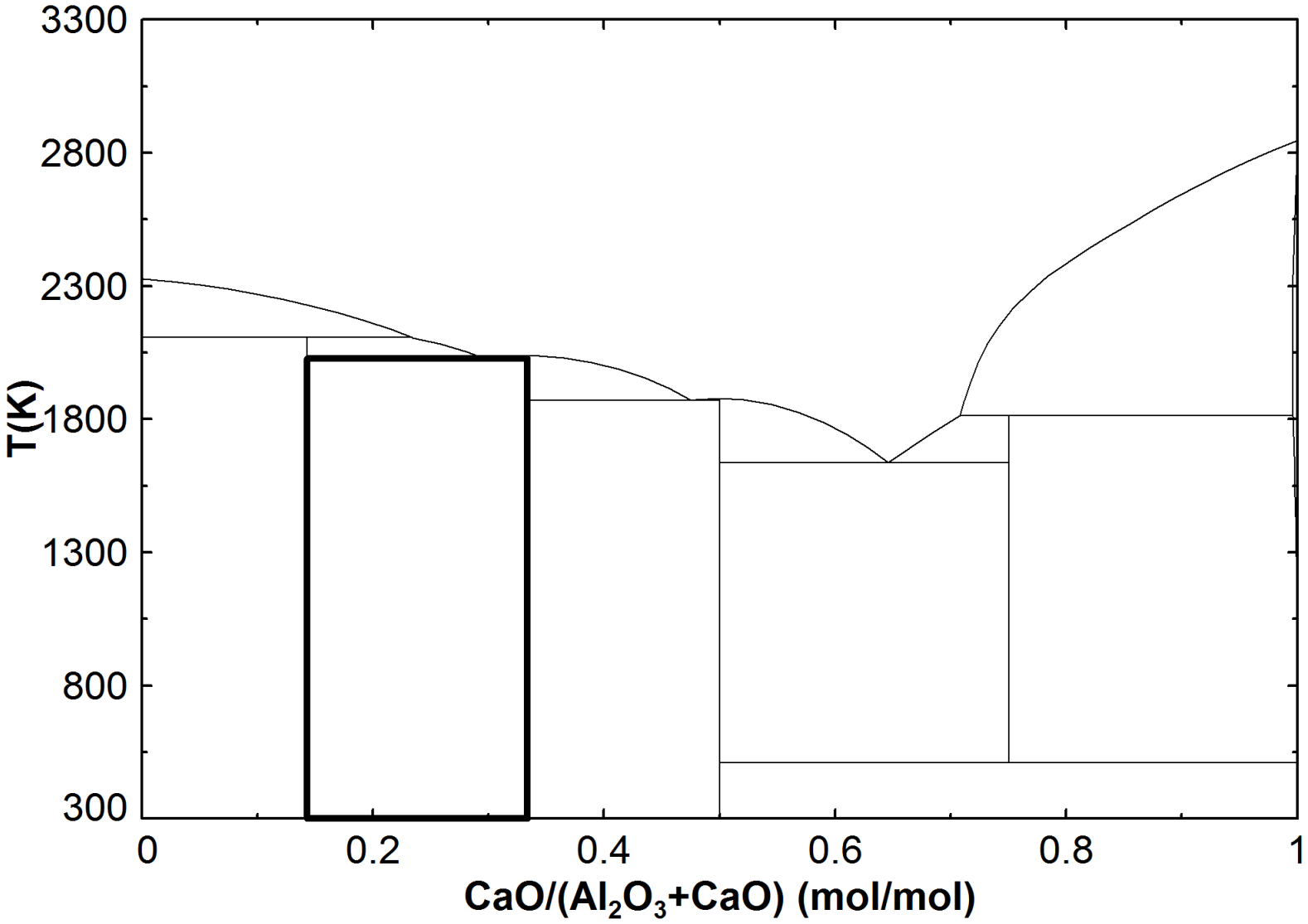
Geometric Approach

- Phase diagrams describe thermochemical behaviour
  - Binary
  - Ternary
- Phase diagrams are also geometric systems, consisting of:
  - Points
  - Phase region boundaries (curves, surfaces)
  - Phase regions (volumes)

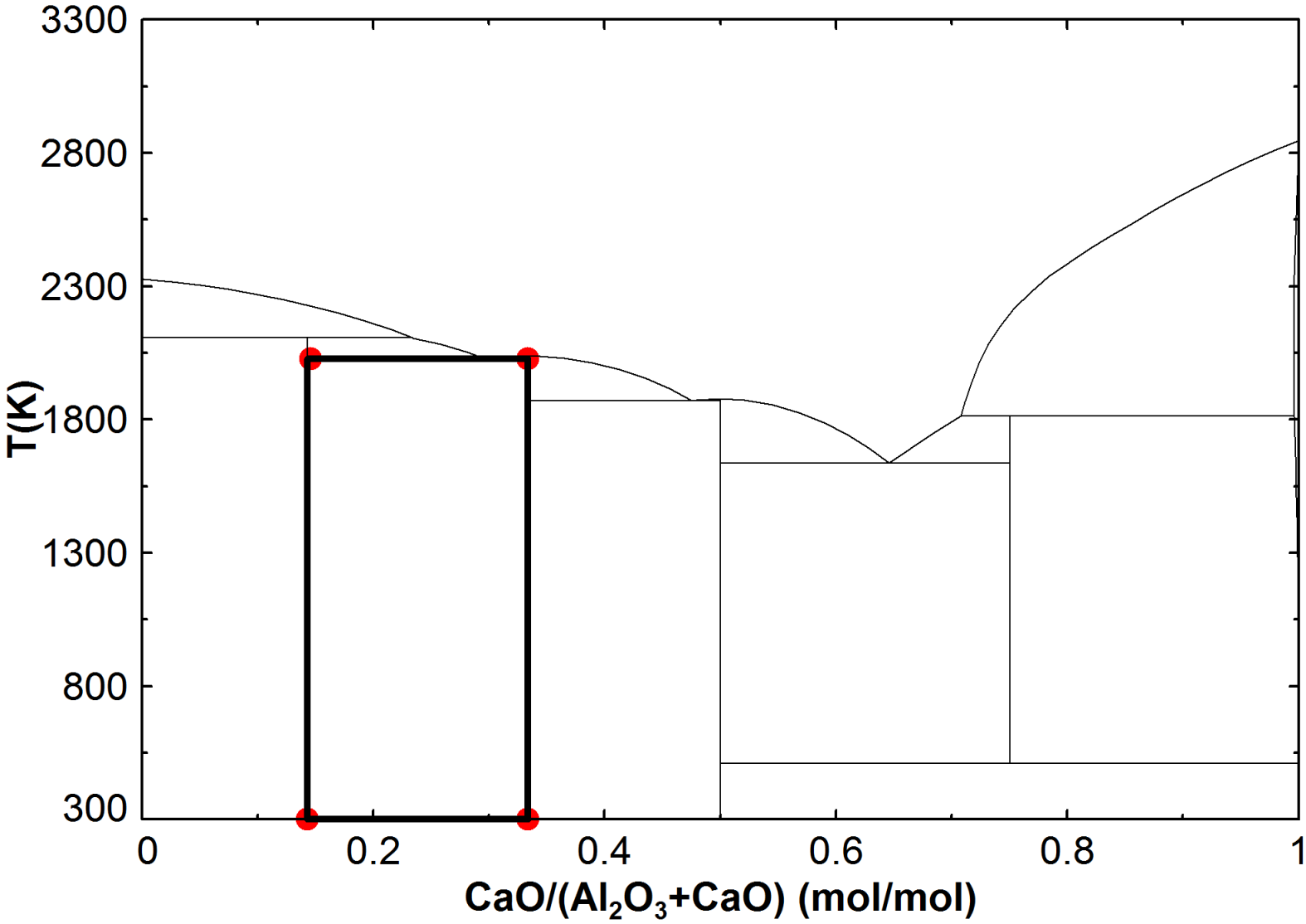
Geometric Approach



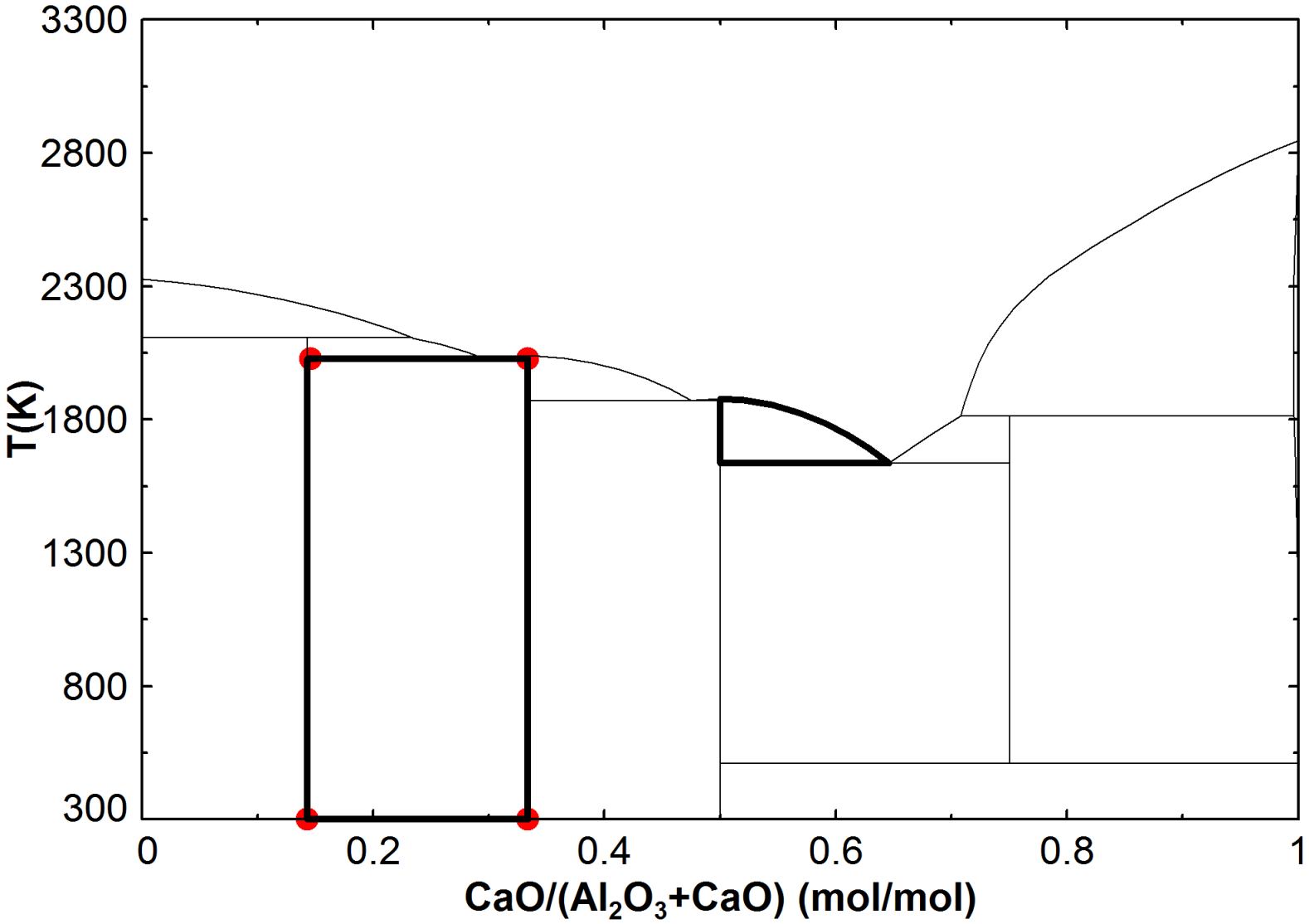
Geometric Approach



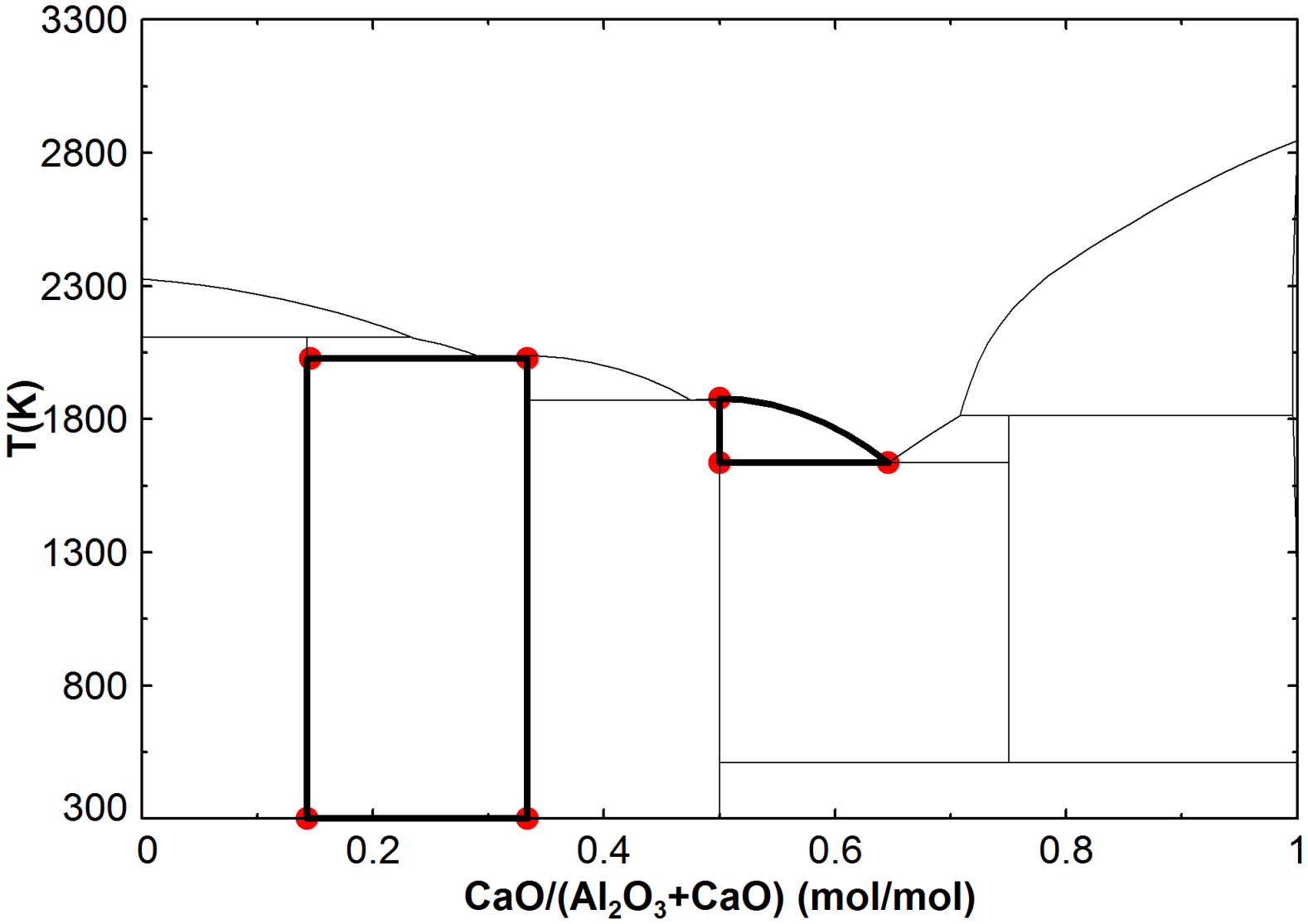
Geometric Approach



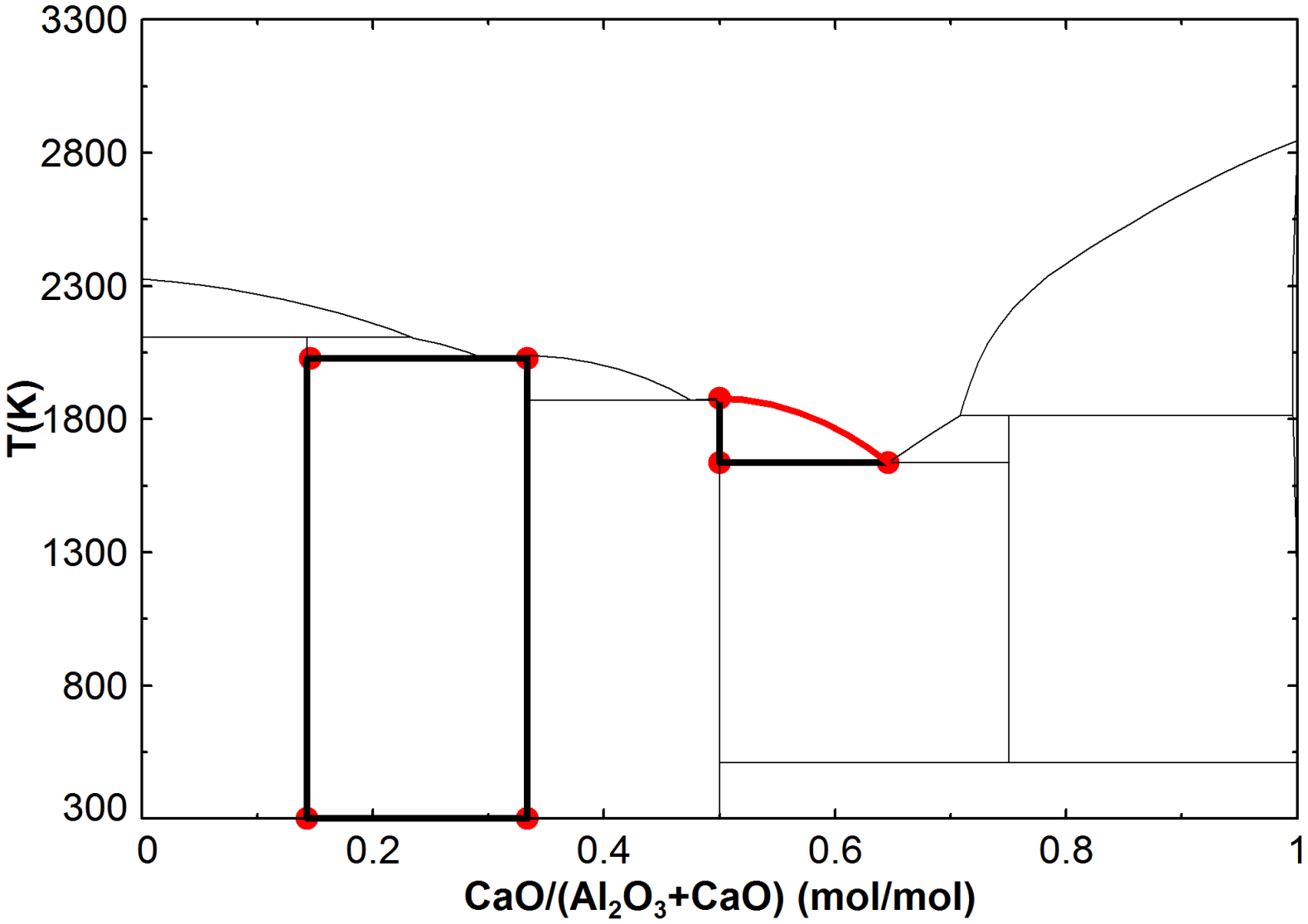
Geometric Approach



Geometric Approach



Geometric Approach



Geometric Approach

Simplifies the calculation of

- Phase fractions
- Phase compositions

Thermochemistry Theory

Gibbs Phase Rule

$$f = c - p + 2$$

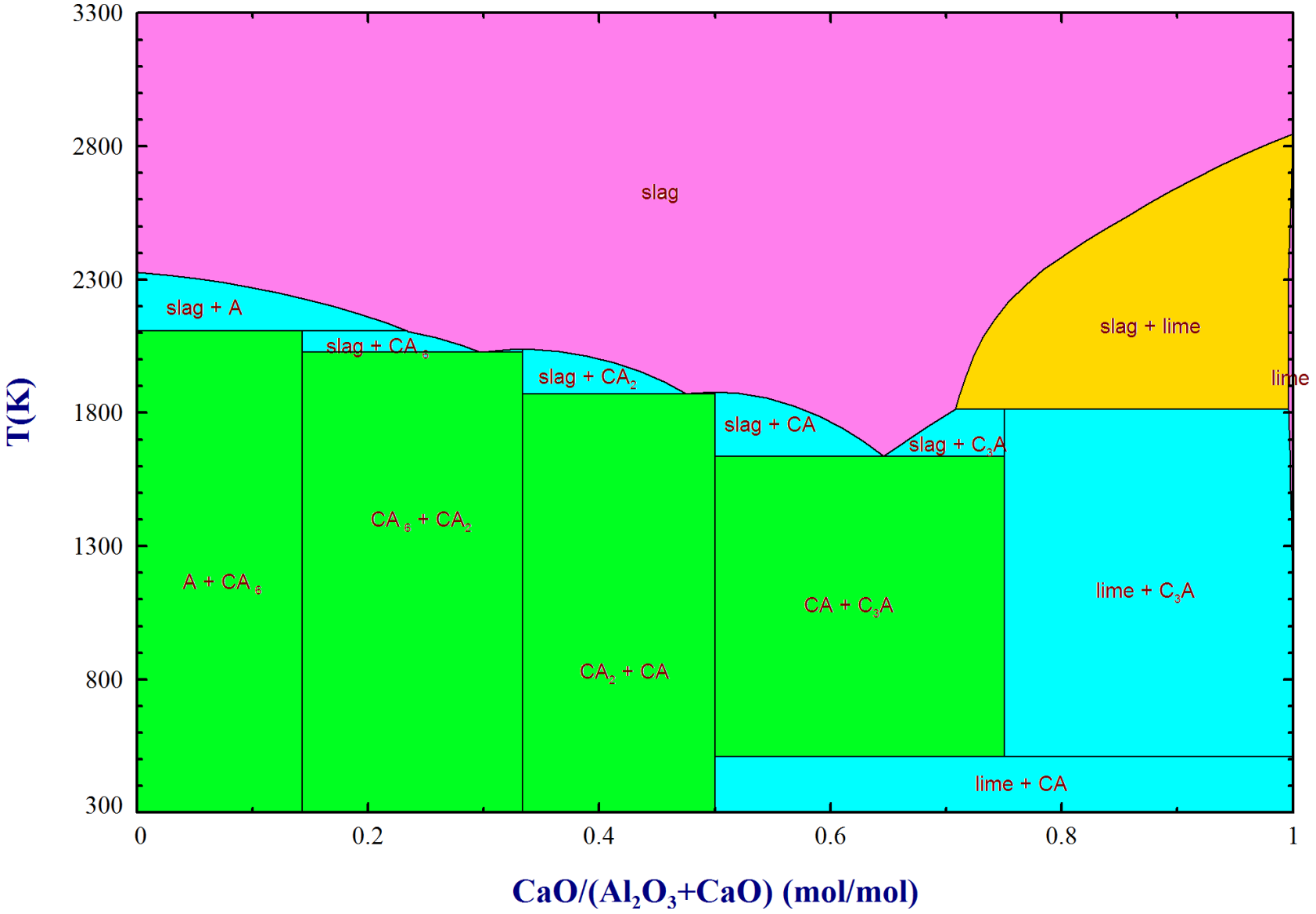
At constant pressure:

$$f' = c - p + 1$$

Classify phase regions

Thermochemistry Theory

Gibbs Phase Rule

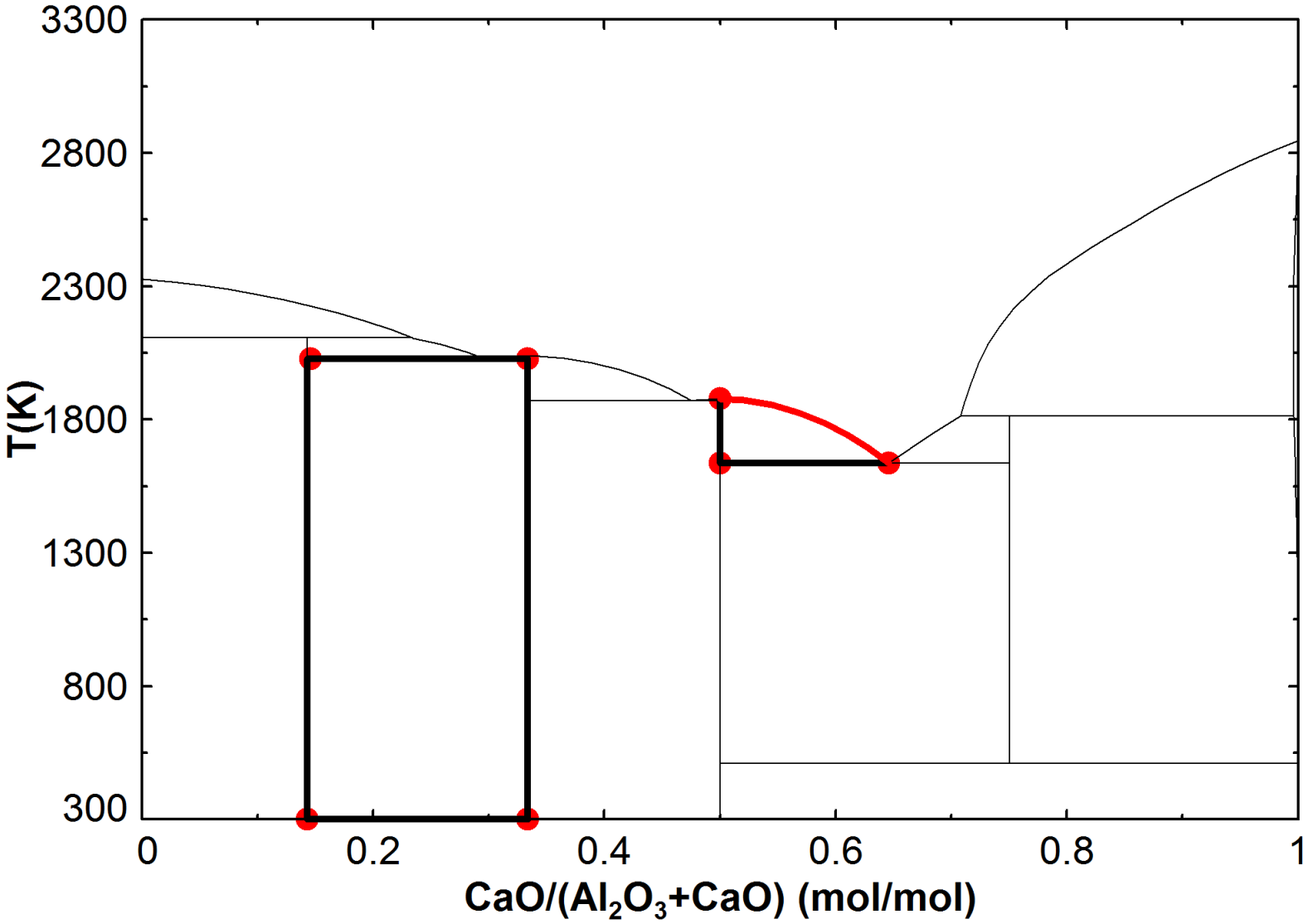


Thermochemistry Theory
Lever Rule

- Reduce dimensionality

Thermochemistry Theory

Lever Rule

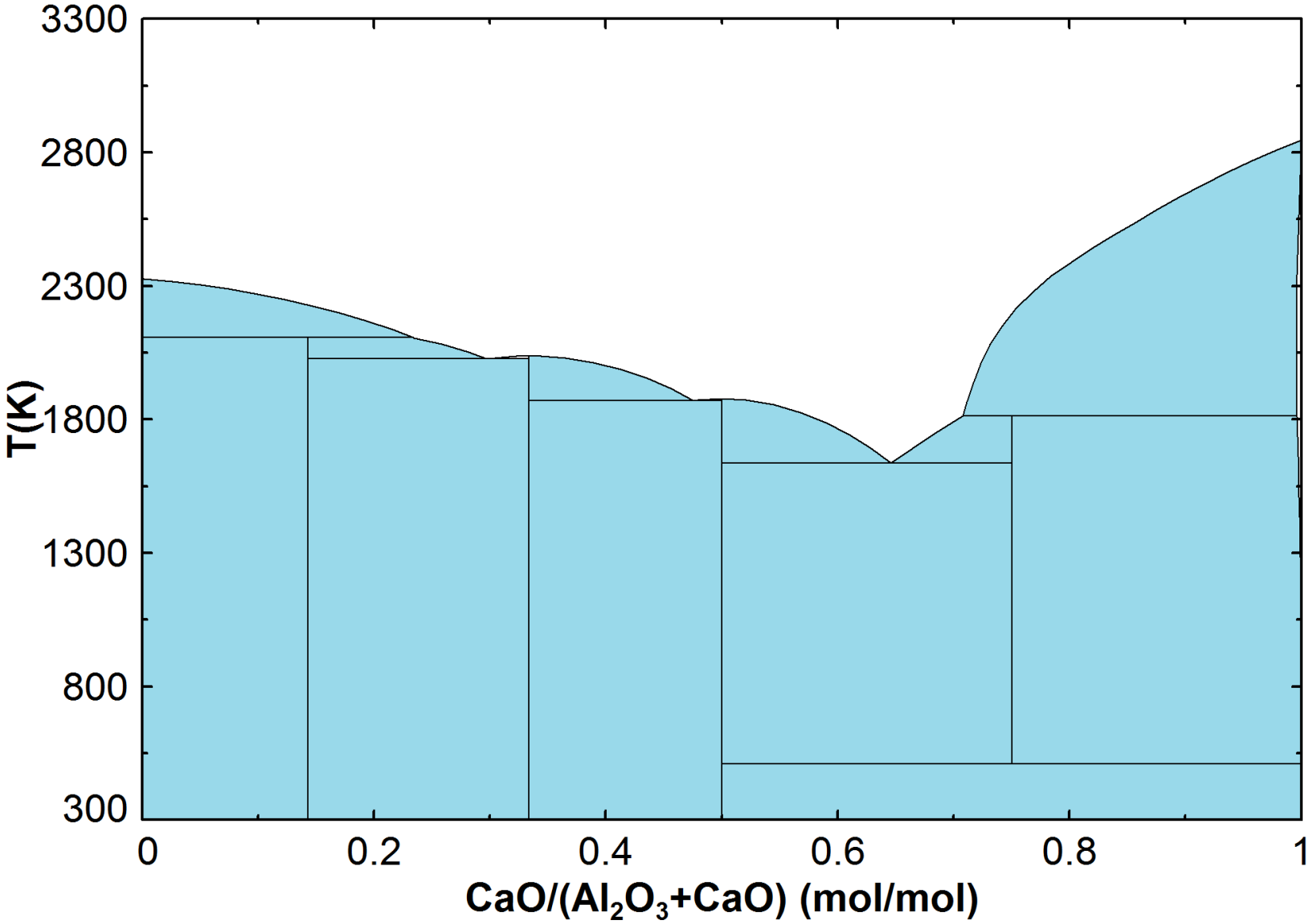


Thermochemistry Theory
Lever Rule

- Reduce dimensionality
- Calculate phase fractions
- Binary systems:
  - 2-phase regions
- Ternary systems:
  - 2-phase regions, 3-phase regions
- c-component systems:
  - 2-phase regions, …, c-phase regions

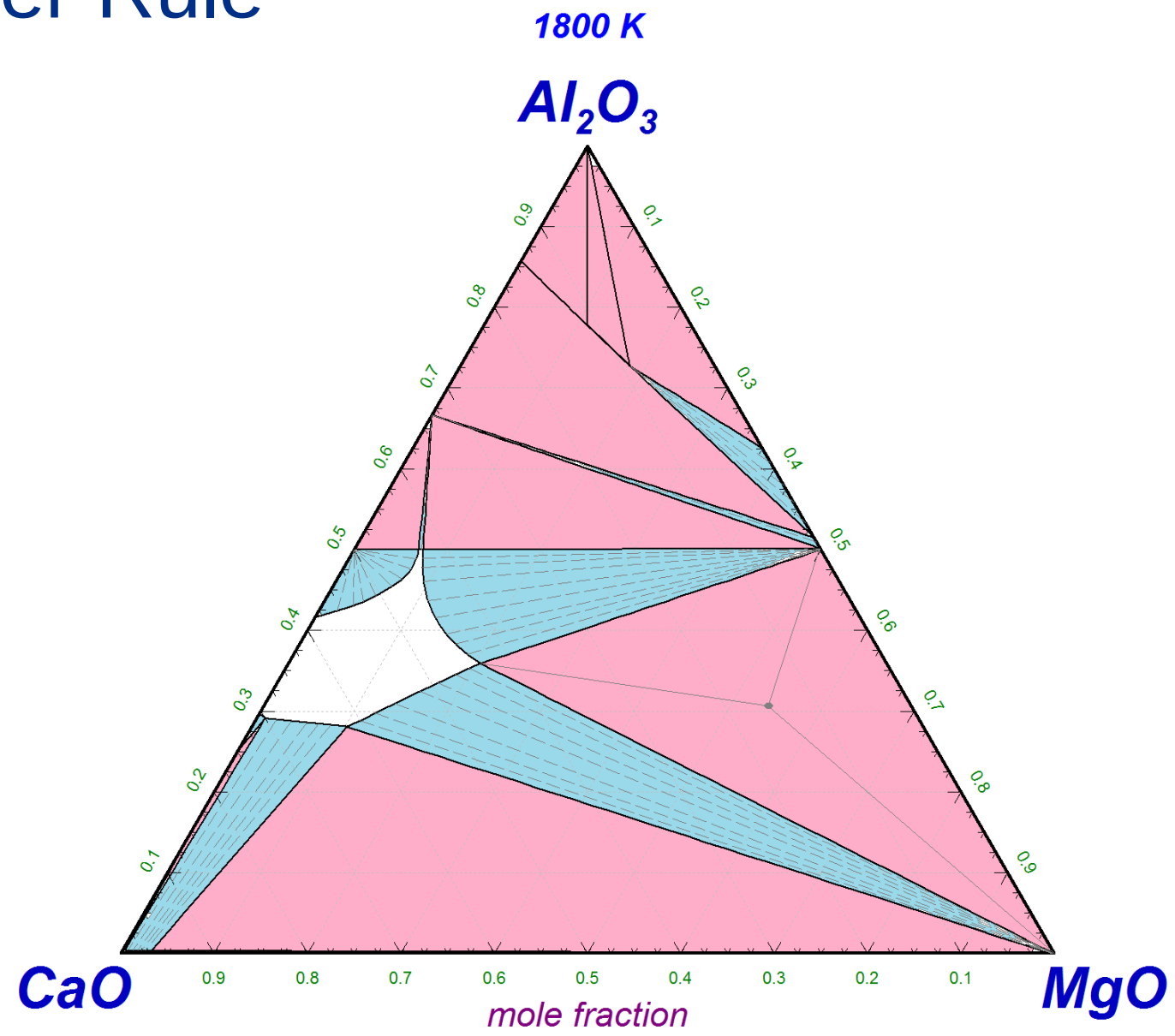
Thermochemistry Theory

Lever Rule



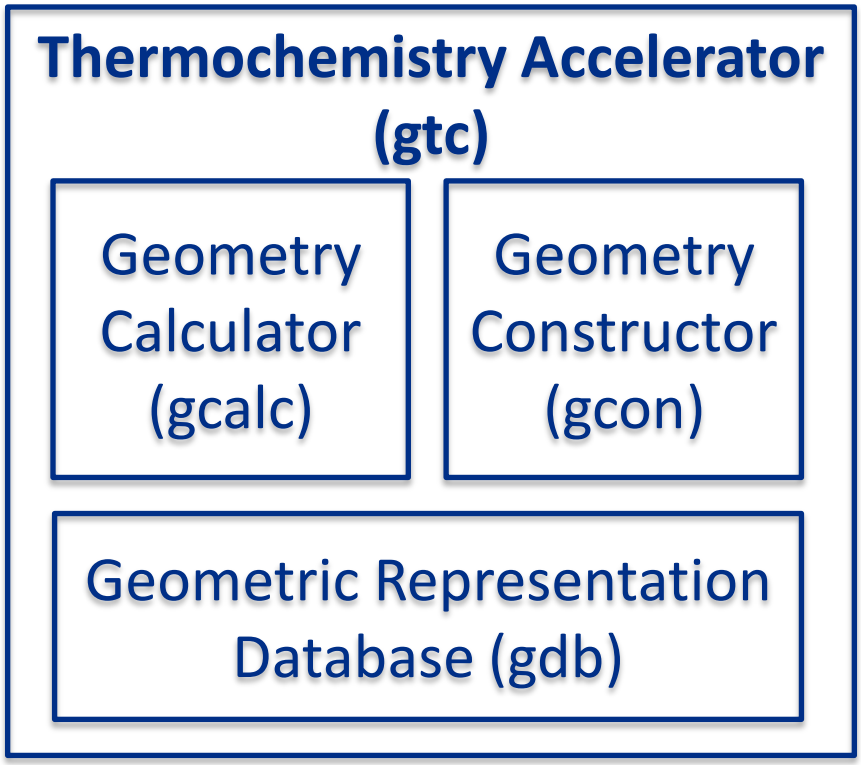
Thermochemistry Theory

Lever Rule



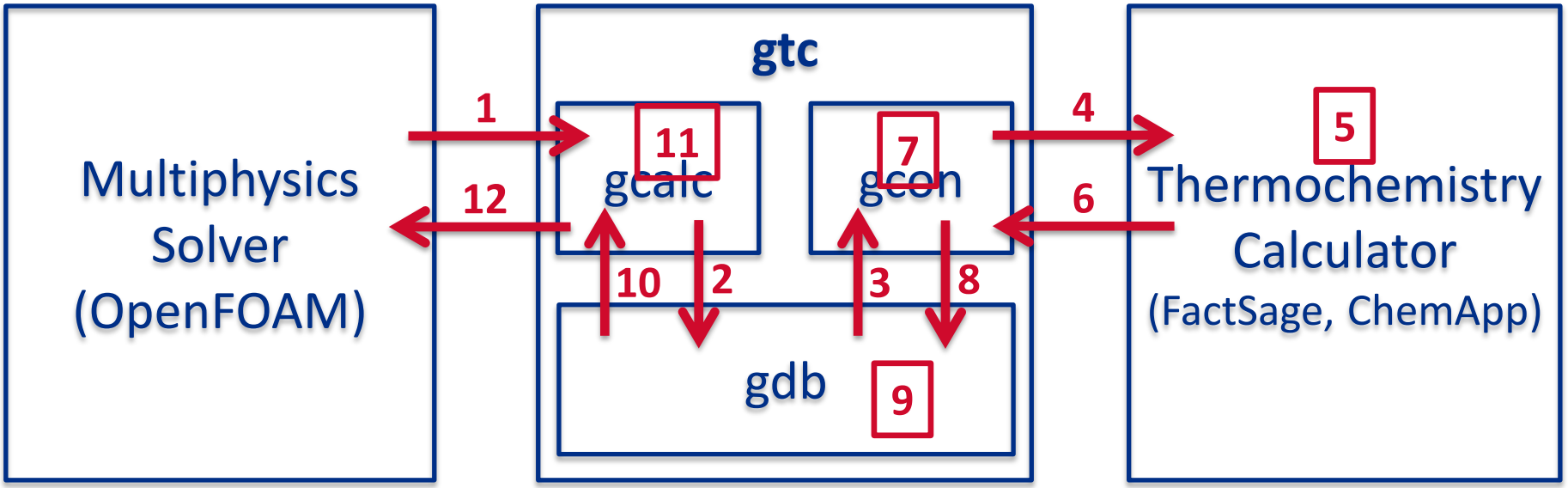
Implementation
Python

- Positive:
  - Extensive mathematical and numerical libraries
  - Simple language
  - Access to ChemApp
  - Rapid prototyping
- Negative:
  - Computationally slow
- Will transfer algorithms to Fortran


Thermochemistry Accelerator (gtc)
Geometry Calculator (gcalc)
Geometry Constructor (gcon)
Geometric Representation Database (gdb)

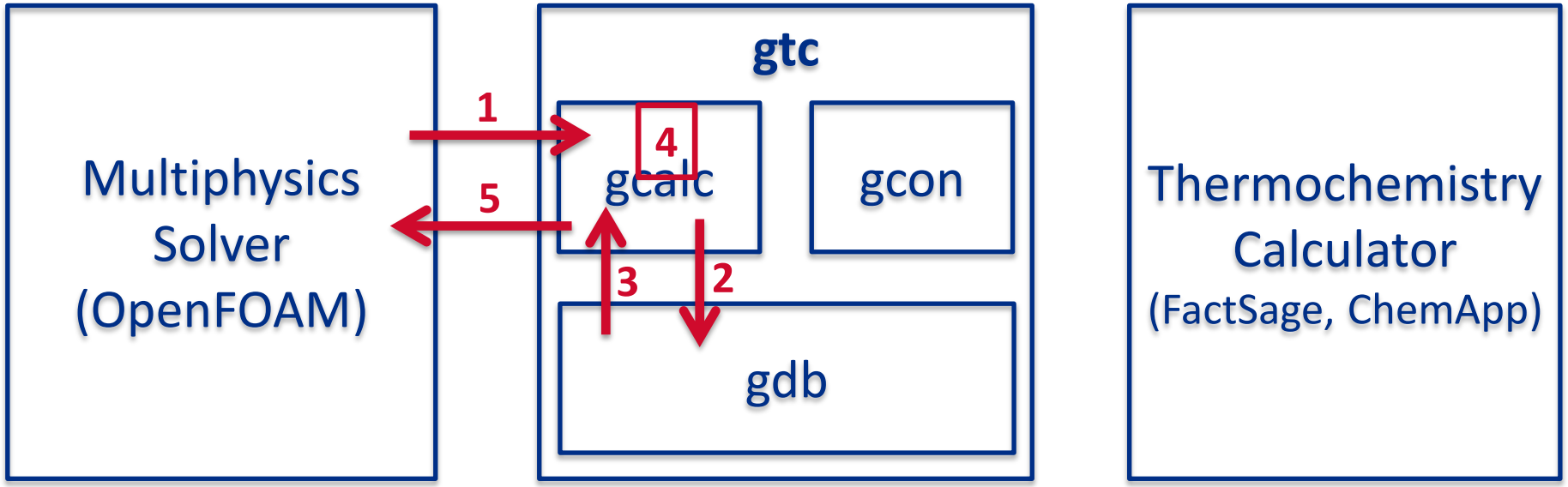
Equilibrium Calculation

New Region



1. request equilibrium result
2. request geometry
3. request geometry construction
4. request equilibrium results
5. do equilibrium calculations
6. provide equilibrium results
7. construct geometry
8. provide geometry
9. store geometry
10. provide geometry
11. calculate equilibrium
12. provide equilibrium result

Equilibrium Calculation
Stored Region



1. request equilibrium result
2. request geometry
3. provide geometry
4. calculate equilibrium
5. provide equilibrium result

Results

Accelerator Performance

- Binary system (Al_2O_3-CaO):
  - 20x faster ChemApp
  - Negligible deviations from ChemApp results
- Ternary (Al_2O_3-CaO-SiO_2):
  - 15x faster than ChemApp
  - Negligible deviations
- Fortran implementation
  - Can be 10x to 1000x faster than Python
  - Possible 150x to 20000x acceleration
  - Multiphysics-thermochemistry integration can become feasible

Next Steps

Future Plans

- Add Cp and H
- Develop generic algorithm for c-component systems
- Develop multicomponent, multiphase solver in OpenFOAM
- Develop test cases
  - Freeze lining
  - Slag-alloy reduction interactions

Thank you