Thermodynamic calculations with a low threshold:

Excel worksheets, 3D phase diagrams, and other educational tools

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GTT workshop 2011

InsPyro

Overview

- Vision
- Excel worksheets
  - Fe-alloy phase calculation
  - Lead battery recycling charge calculation
- Whiteboard
- 3D phase diagram printing
- Conclusions

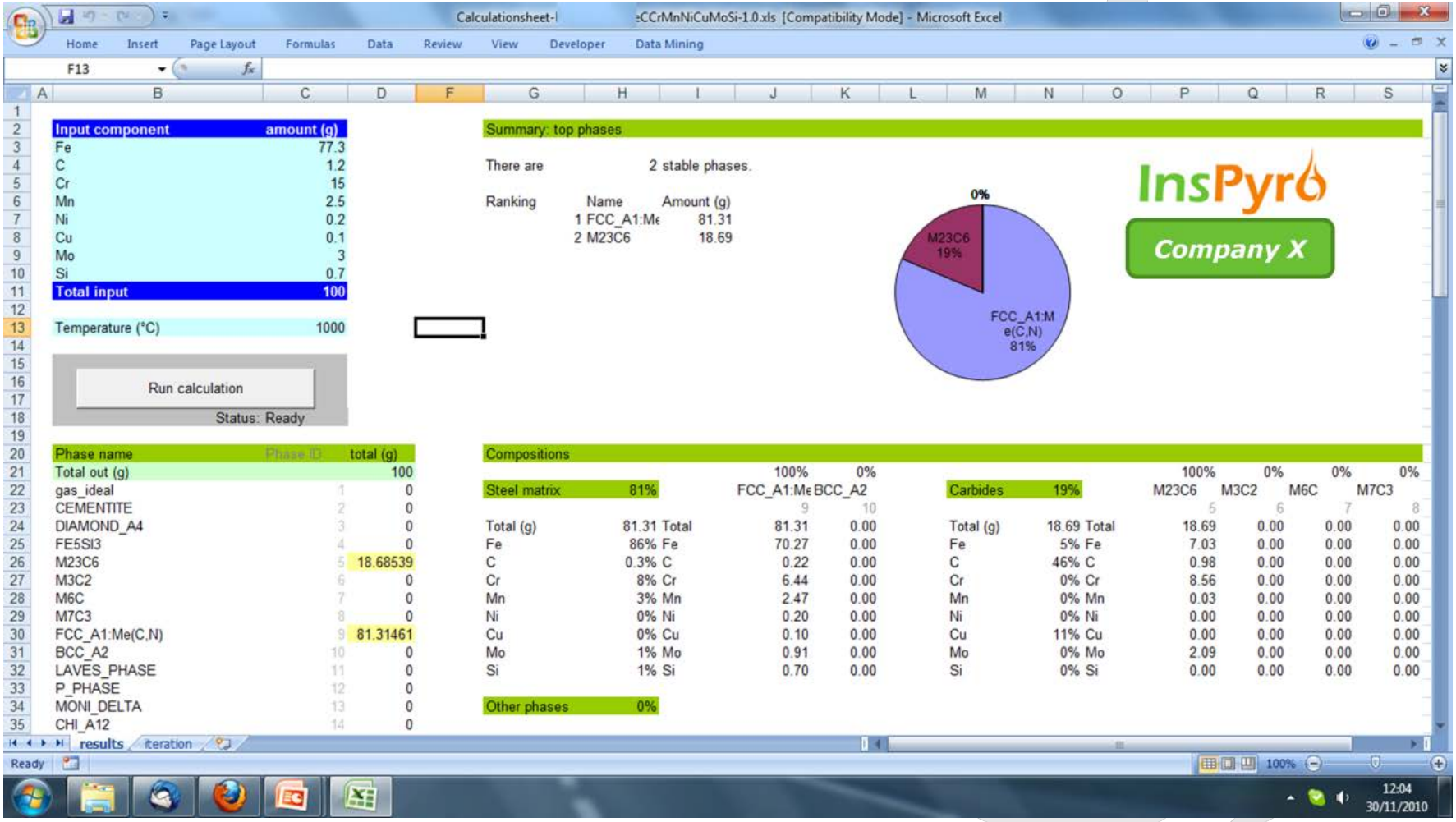
Vision

- Thermodynamics are powerful
- However, (even) FactSage is not so user friendly:
  - Selection of phases:
    - Overlapping databases/models
    - Metastability
    - Missing compounds or components
    - Updates
  - Own logic of calculation set-up
- Metallurgy and related industry need simpler way to access complicated models

+ All help to understand phase diagrams is welcome

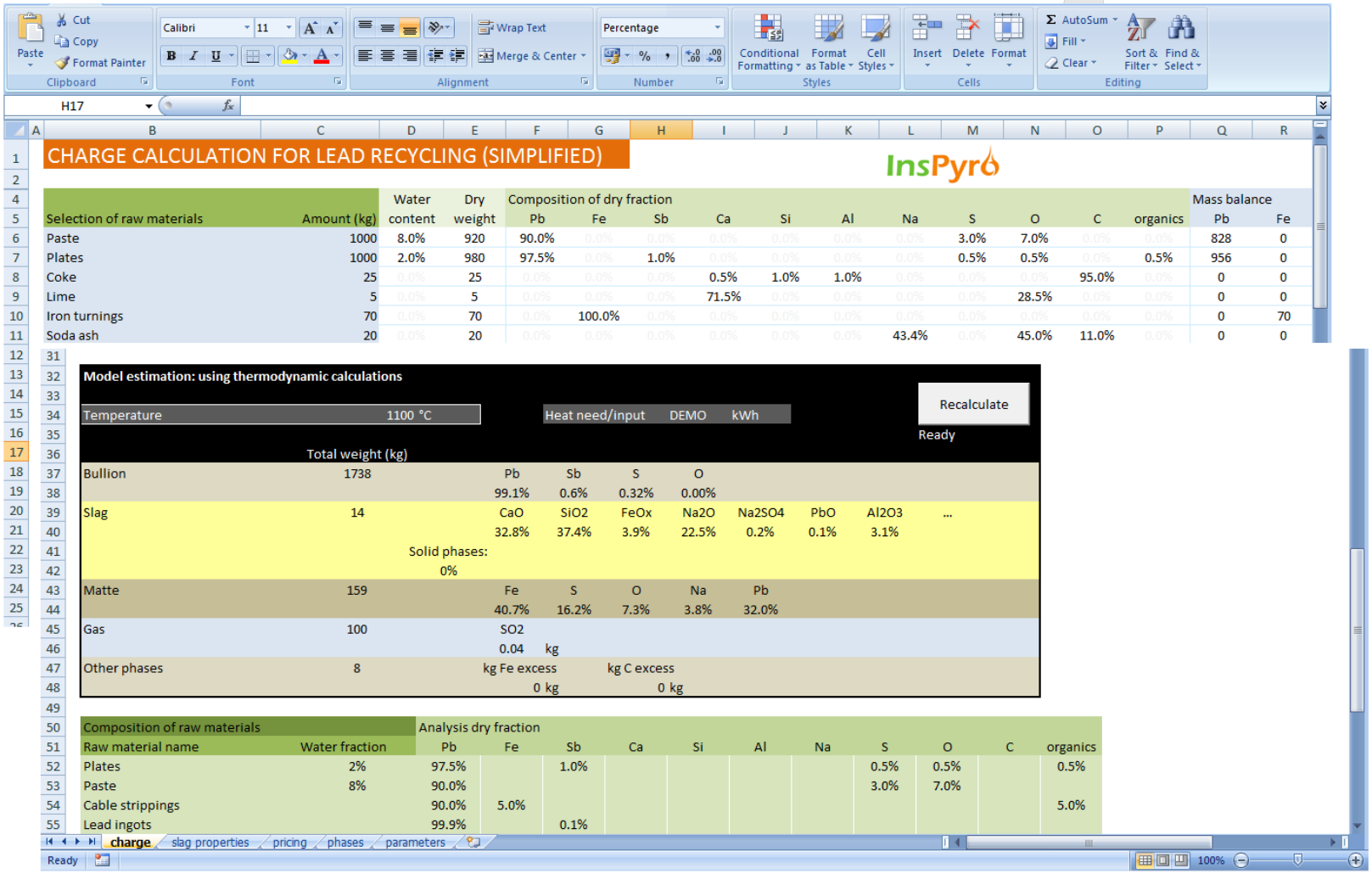
Excel calculation sheets

- Example 1: Fe-alloy



Excel calculation sheets

- Example 2: Lead recycling



CHARGE CALCULATION FOR LEAD RECYCLING (SIMPLIFIED)

InsPyro

Selection of raw materials	Amount (kg)	Water content	Dry weight	Composition of dry fraction Pb	Fe	Sb	Ca	Si	Al	Na	S	O	C	organics	Mass balance Pb	Fe
Paste	1000	8.0%	920	90.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	3.0%	7.0%	0.0%	0.0%	828	0
Plates	1000	2.0%	980	97.5%	0.0%	1.0%	0.0%	0.0%	0.0%	0.0%	0.5%	0.5%	0.0%	0.5%	956	0
Coke	25	0.0%	25	0.0%	0.0%	0.0%	0.5%	1.0%	1.0%	0.0%	0.0%	0.0%	95.0%	0.0%	0	0
Lime	5	0.0%	5	0.0%	0.0%	0.0%	71.5%	0.0%	0.0%	0.0%	0.0%	28.5%	0.0%	0.0%	0	0
Iron turnings	70	0.0%	70	0.0%	100.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0	70
Soda ash	20	0.0%	20	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	43.4%	0.0%	45.0%	11.0%	0.0%	0	0

Model estimation: using thermodynamic calculations

Temperature 1100 °C

Heat need/input DEMO kWh

Recalculate

Ready

	Total weight (kg)								
Bullion	1738	Pb 99.1%	Sb 0.6%	S 0.32%	O 0.00%				
Slag	14	CaO 32.8%	SiO2 37.4%	FeOx 3.9%	Na2O 22.5%	Na2SO4 0.2%	PbO 0.1%	Al2O3 3.1%	...
	Solid phases: 0%								
Matte	159	Fe 40.7%	S 16.2%	O 7.3%	Na 3.8%	Pb 32.0%			
Gas	100	SO2 0.04 kg							
Other phases	8	kg Fe excess 0 kg		kg C excess 0 kg					

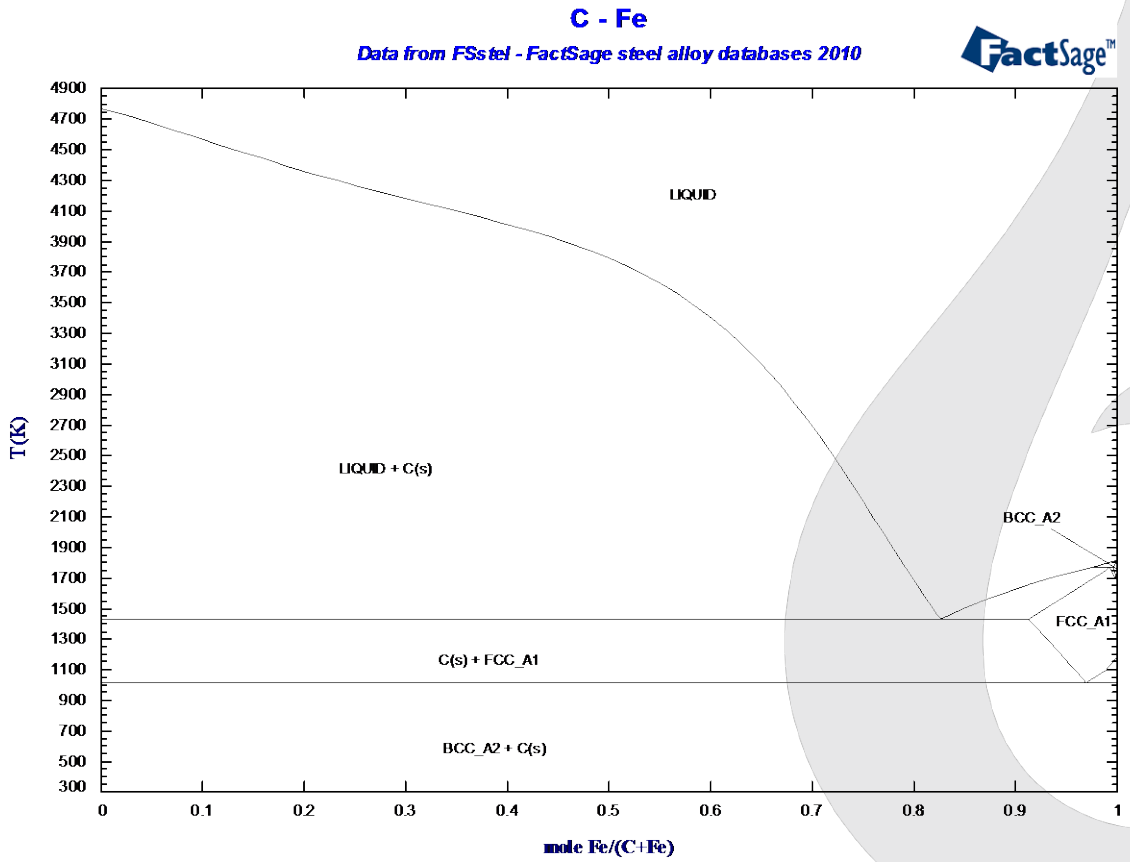
Composition of raw materials		Analysis dry fraction										
Raw material name	Water fraction	Pb	Fe	Sb	Ca	Si	Al	Na	S	O	C	organics
Plates	2%	97.5%		1.0%					0.5%	0.5%		0.5%
Paste	8%	90.0%							3.0%	7.0%		
Cable strippings		90.0%	5.0%									5.0%
Lead ingots		99.9%		0.1%								

charge | slag properties | pricing | phases | parameters

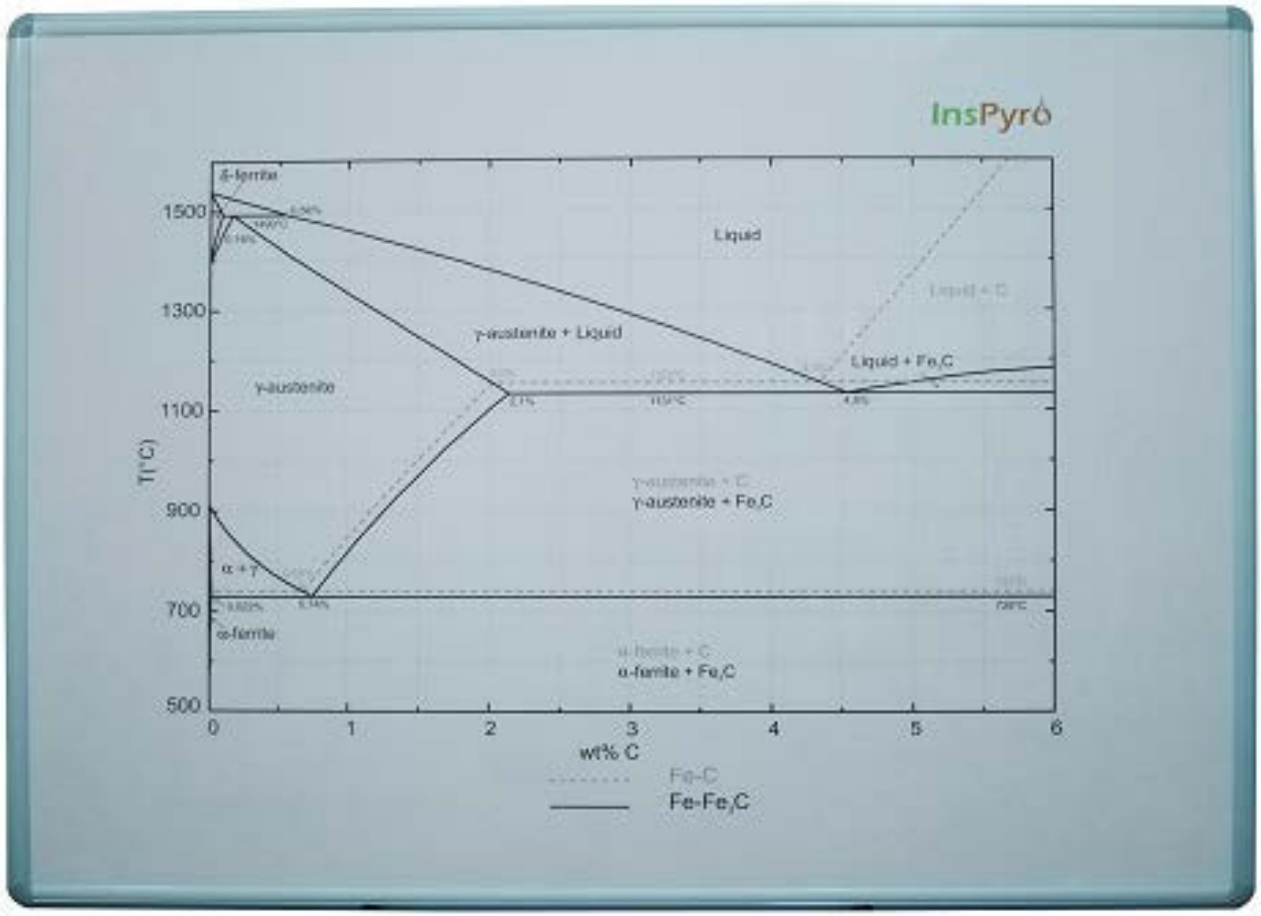
Ready 100%

Phase diagram whiteboards

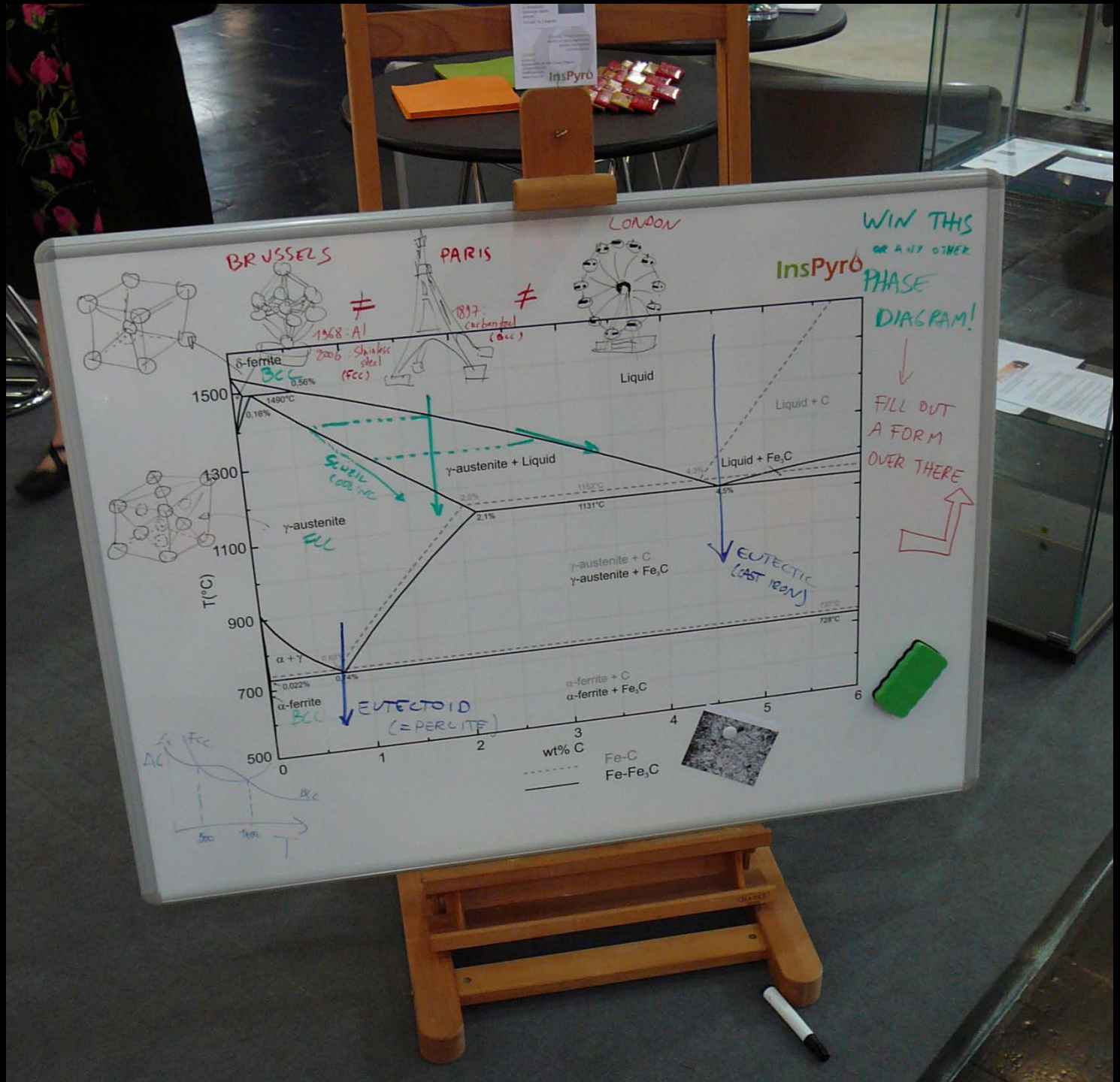
- A classic: the Fe-C diagram



Put it on a whiteboard...



- … and it comes to life!


BRUSSELS
PARIS
LONDON
WIN THIS
OR ANY OTHER
InsPyro
PHASE
DIAGRAM!
FILL OUT
A FORM
OVER THERE
1968 : Al
2006 : Stainless steel (FCC)
1897 : carbon steel (BCC)
δ-ferrite
BCC
0.56%
1490°C
0.16%
Liquid
Liquid + C
γ-austenite + Liquid
Liquid + Fe3C
4.3%
1152°C
2.0%
2.1%
1131°C
4.5%
γ-austenite
FCC
γ-austenite + C
γ-austenite + Fe3C
EUTECTIC
(CAST IRON)
T(°C)
1500
1300
1100
900
700
500
α + γ
0.022%
0.74%
728°C
α-ferrite
BCC
α-ferrite + C
α-ferrite + Fe3C
EUTECTOID
(=PERLITE)
0
1
2
3
4
5
6
wt% C
Fe-C
Fe-Fe3C
ΔC
FCC
BCC


BRUSSELS
PARIS


γ-austenite + C
γ-austenite + Fe3C
α-ferrite + C
α-ferrite + Fe3C
2
3
4
5
6
wt% C
Fe-C
Fe-Fe3C

3D phase diagrams

- Liquidus projections can be difficult to imagine at first
- 3D examples used in education are helpful, but mainly for theoretical, ideal systems
- With a real system, it can be a discussion tool as well (and an eye catcher)

- Rapid manufacturing techniques can produce any shape – so why not a phase diagram?

Ag-Pb-Zn ternary liquidus projection

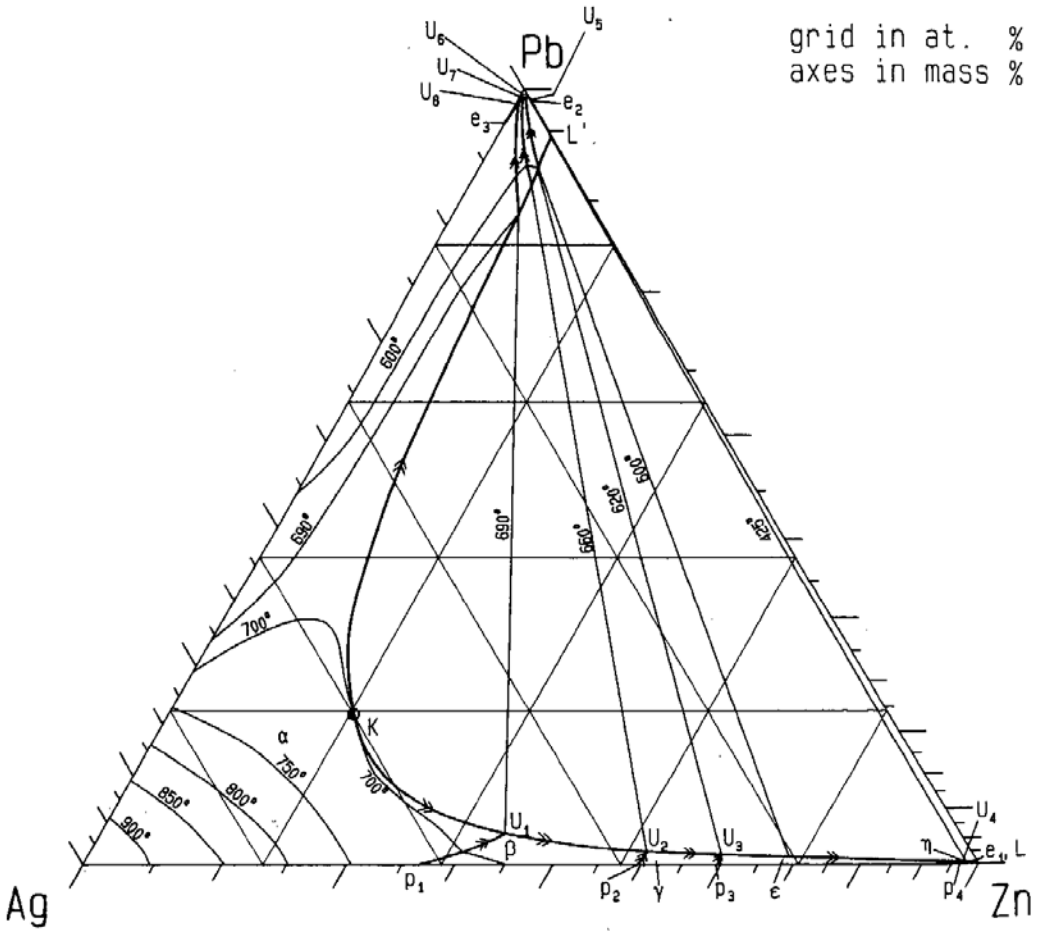


Figure 2: Liquidus surface and tie lines (miscibility gap).

Kubaschewski

Ag-Pb-Zn miscibility gap

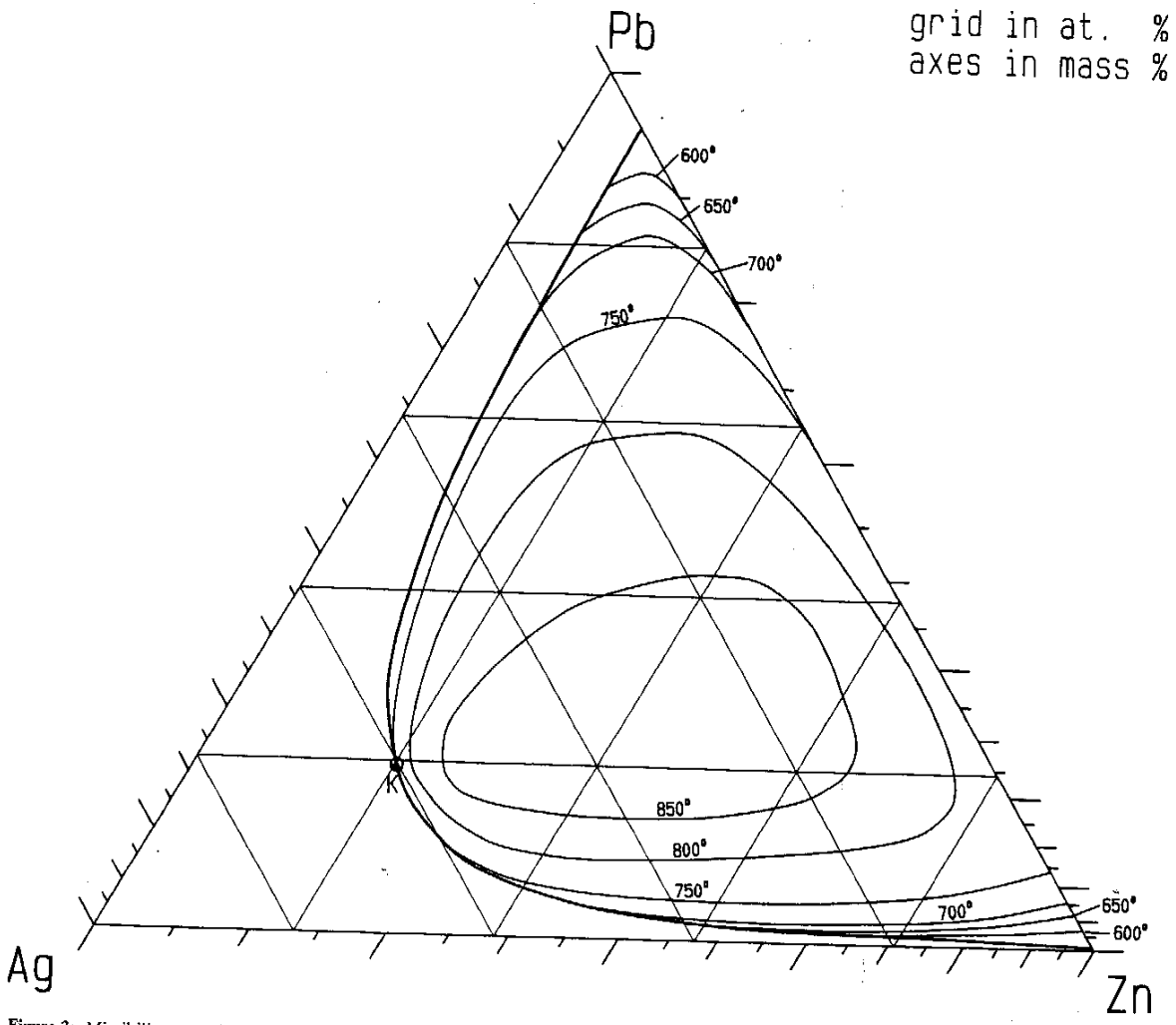
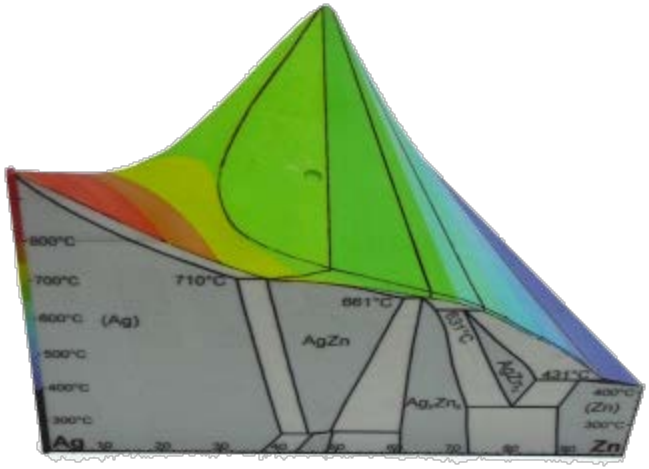


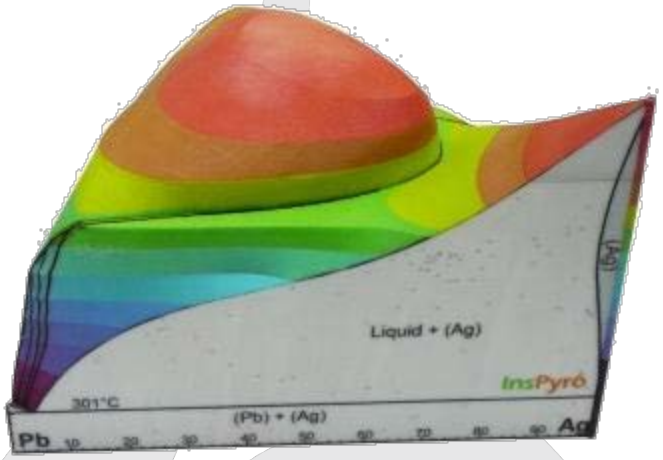
Figure 3: Miscibility gap : liquid state isothermals.

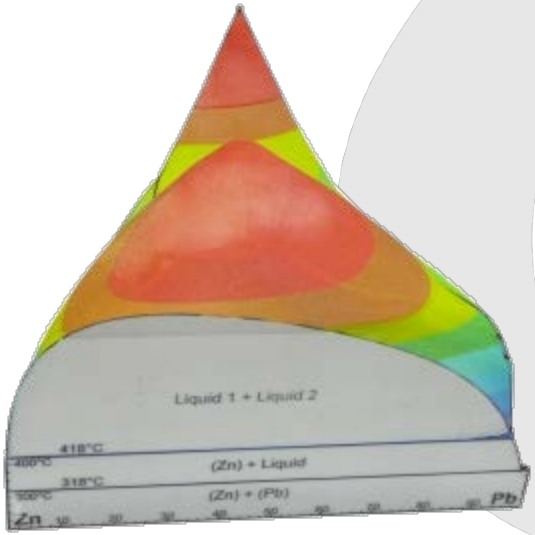
First step: digital 3D model

- 3D model

Second step: physical 3D model





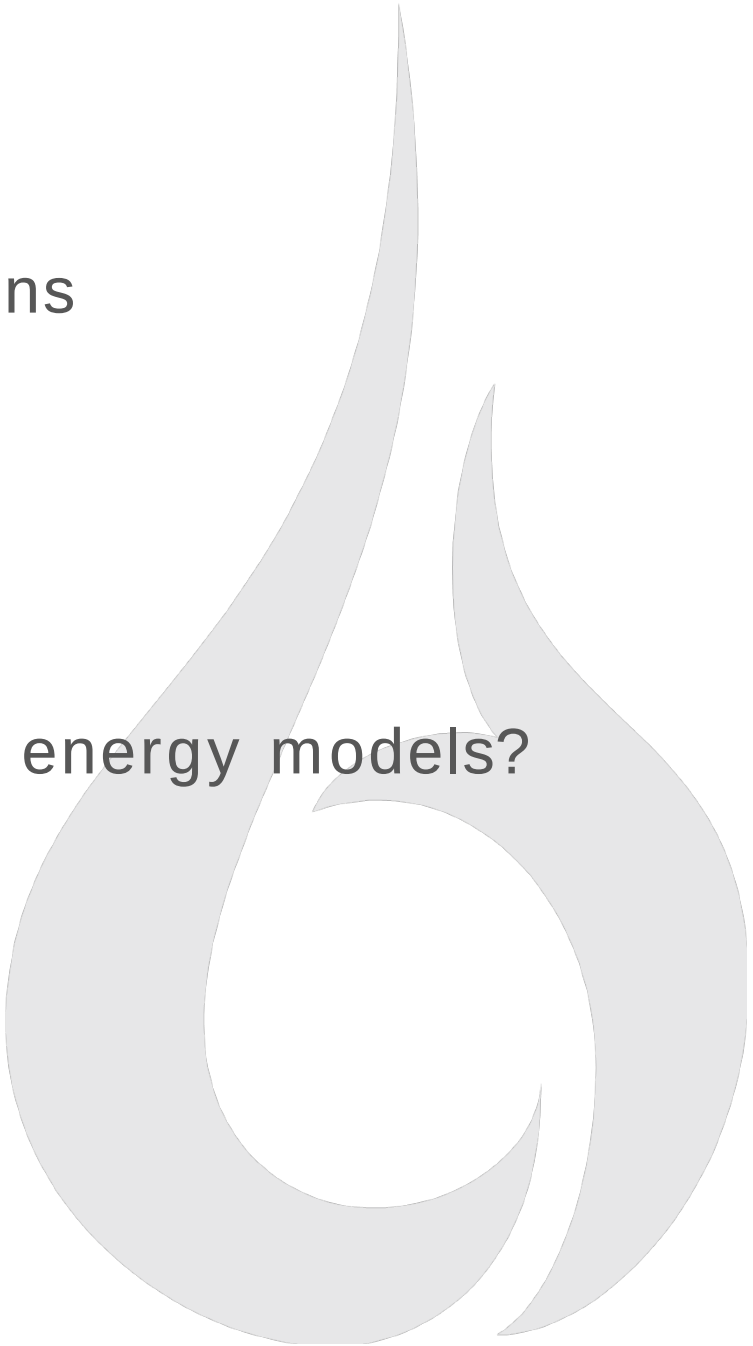



Liquid 1 + Liquid 2
(Zn) + Liquid
(Zn) + (Pb)
(Sn) + (Sb)
(Sn) + Pb3Sn
Pb3Sn + Pb3Sn_2
Pyro

Improvements

- Vertical and horizontal sections
- Phase volume puzzle
- Transparency?

- Improved smoothness
- 3D modelling from the Gibbs energy models?



Conclusions

- Using well-known spreadsheets to make thermodynamics easier…
  - Point calculations for stable phase in alloy
  - Simple effect of composition or T influences
  - Integrate in charge calculation
- Using new techniques to make thermodynamics tangible…
  - Writable whiteboard of any system
  - Full colour 3D print of any system
- InsPyro always tries to simplify the answer, without simplifying the question!