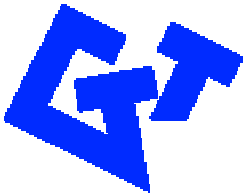


ChemSheet Introduction

Karri Penttilä and Pertti Koukkari, VTT

GTT Workshop, Herzogenrath, Germany, May 17-19, 2006

Introduction

- **Chemsheet** works as an add-in program of general thermodynamics in **Excel**.
- The thermochemical programming library **ChemApp** is used in combination with its application-specific thermochemical data.
- The non-ideal solution models cover concentrated aqueous solutions, dilute and concentrated alloys, liquid slags and molten salts, solid solutions, non-ideal gases and non-stoichiometric systems.
- ChemSheet is straightforward and easy to use and requires no programming skills other than normal Excel use.
- To the user, the process model can be just one Excel-file.

Definition of Terms

- A thermodynamic **system** consists of a number of **phases**. Phases are divided into three groups - the gaseous phase, mixture phases, and invariant phases.
- Phases have one or more **constituents**. Phase constituents have compositions expressed as amounts of a number of **components**.
- A component is a system-wide entity. Usually components are elements, but it is also possible for them to be stoichiometric combinations of elements. For example, in an oxide system based on *calcia* and *silica*, *CaO* and SiO_2, may be used, as well as *Ca*, *Si*, and *O*.

Initial Conditions

- Two different methods are available:
  - Using **Global conditions** of the System
  - Using **Streams**

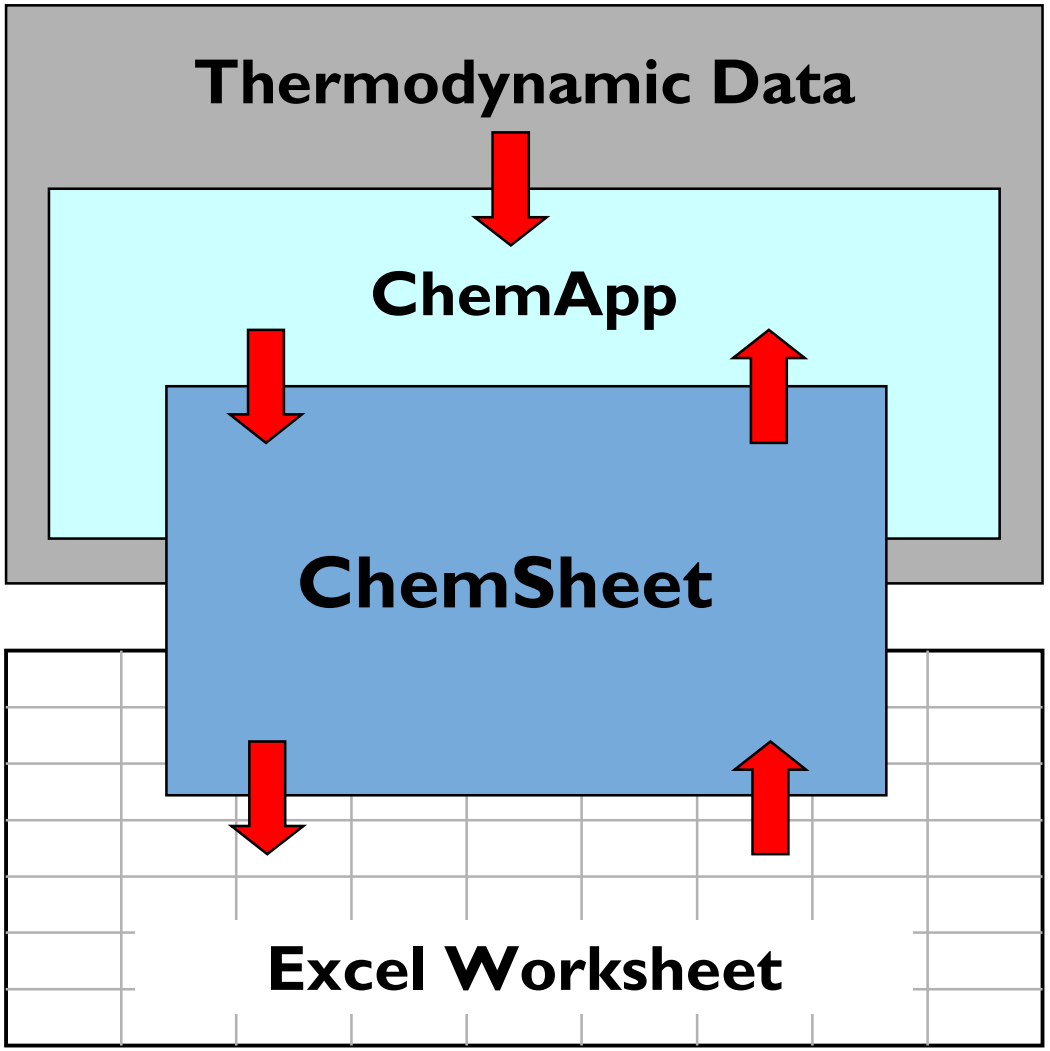
Using Global conditions, you merely need to set single values for temperature and pressure, and enter incoming constituents to define the initial composition of the system.

A stream is a means for transferring non-reacted matter to a reaction zone. It has constant temperature and pressure, and contains one or more constituents. When using **Streams**, you set the three variables: – temperature, pressure and composition for each input stream and set single conditions for temperature and pressure of the system

Using Targets

- **Chemsheet** works as an add-in program of general thermodynamics in **Excel**.
- The thermochemical programming library **ChemApp** is used in combination with its application-specific thermochemical data.
- The non-ideal solution models cover concentrated aqueous solutions, dilute and concentrated alloys, liquid slags and molten salts, solid solutions, non-ideal gases and non-stoichiometric systems.
- ChemSheet is straightforward and easy to use and requires no programming skills other than normal Excel use.
- To the user, the process model can be just one Excel-file.

ChemSheet Interactions



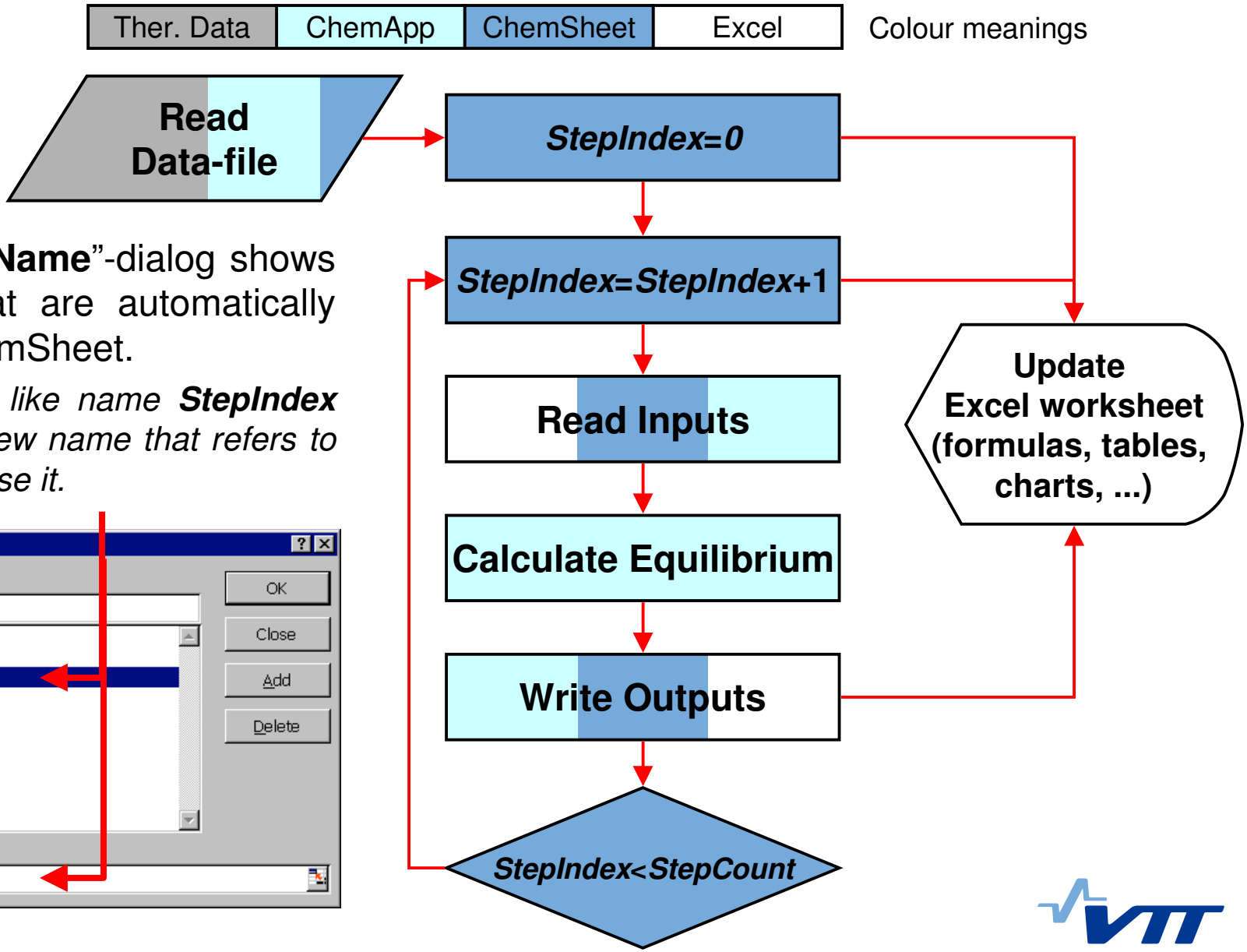
Multi-phase thermodynamics

- alloys and steels
- liquid slags and molten salts
- solid oxides, sulphides and salts
- non-stoichiometric solids
- concentrated aqueous solutions
- pulp suspensions

Using macros in Excel

- heat transfer
- mass transfer (flow, diffusion etc.)
- reaction kinetics
- applied phase-diagrams
- process simulation and characteristics
- spreadsheet modeling of complex phenomena

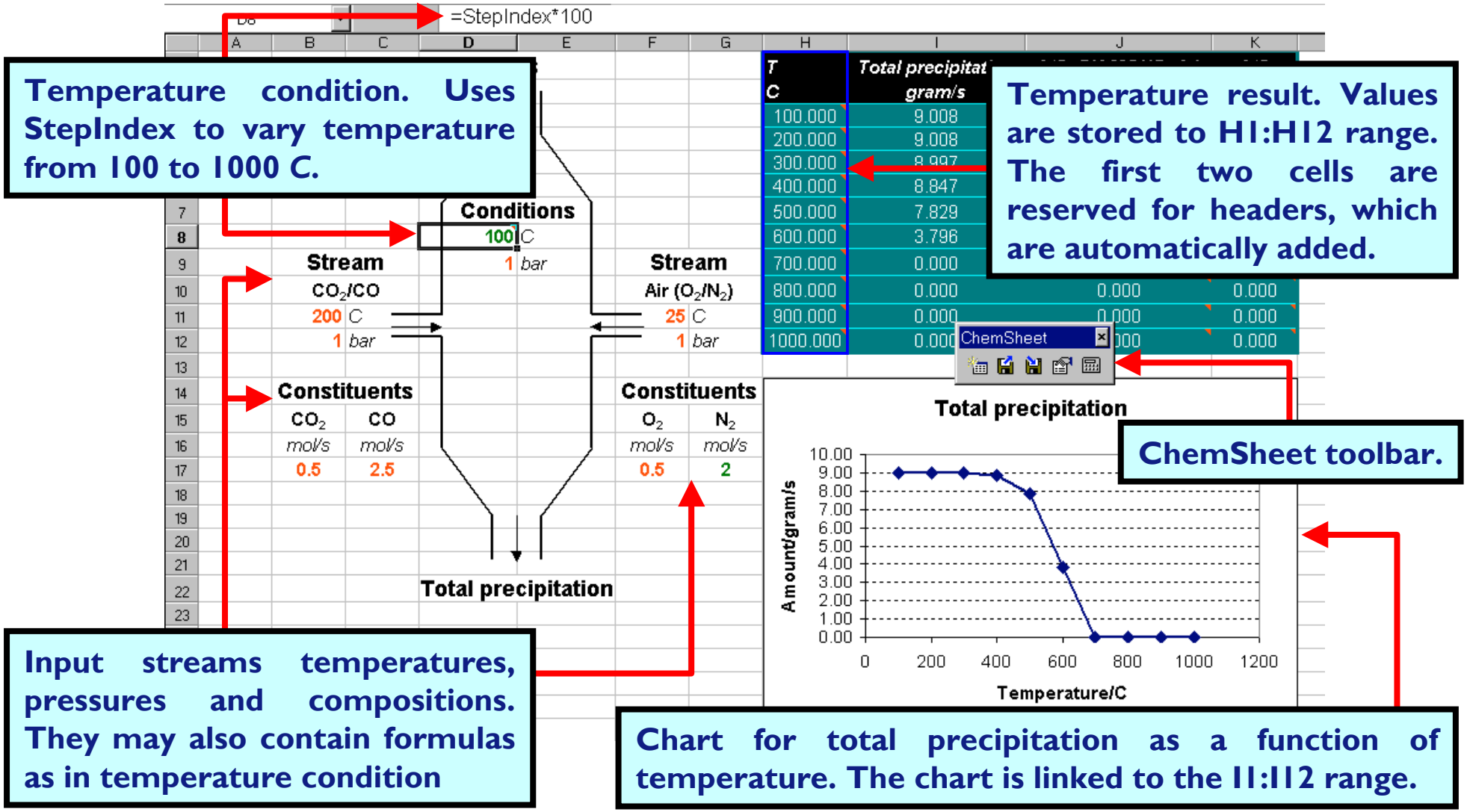
ChemSheet Principle



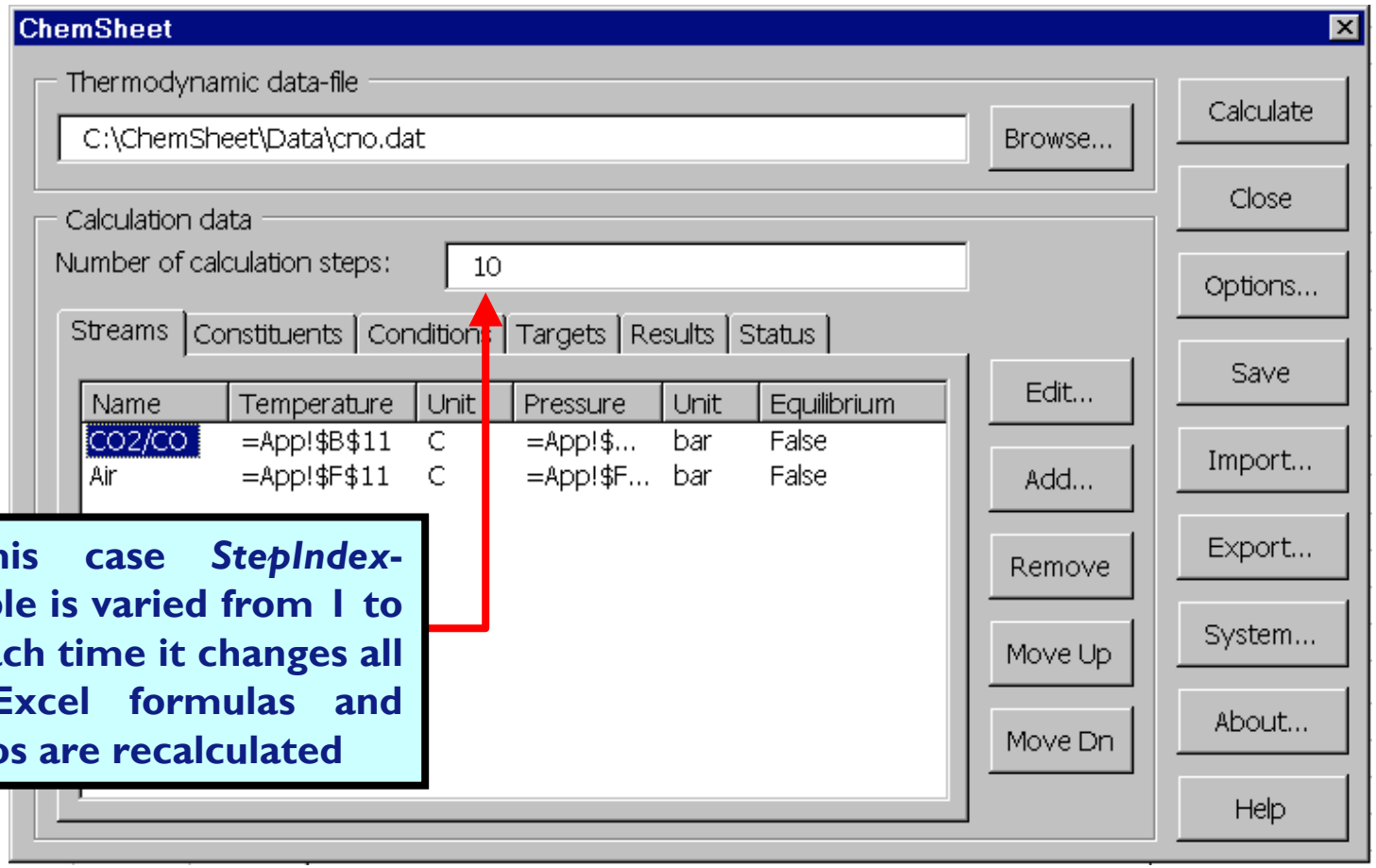
Excel "**Define Name**"-dialog shows the names that are automatically defined by ChemSheet.

Tip *If you don't like name* ***StepIndex*** *you can add a new name that refers to* ***StepIndex*** *and use it.*

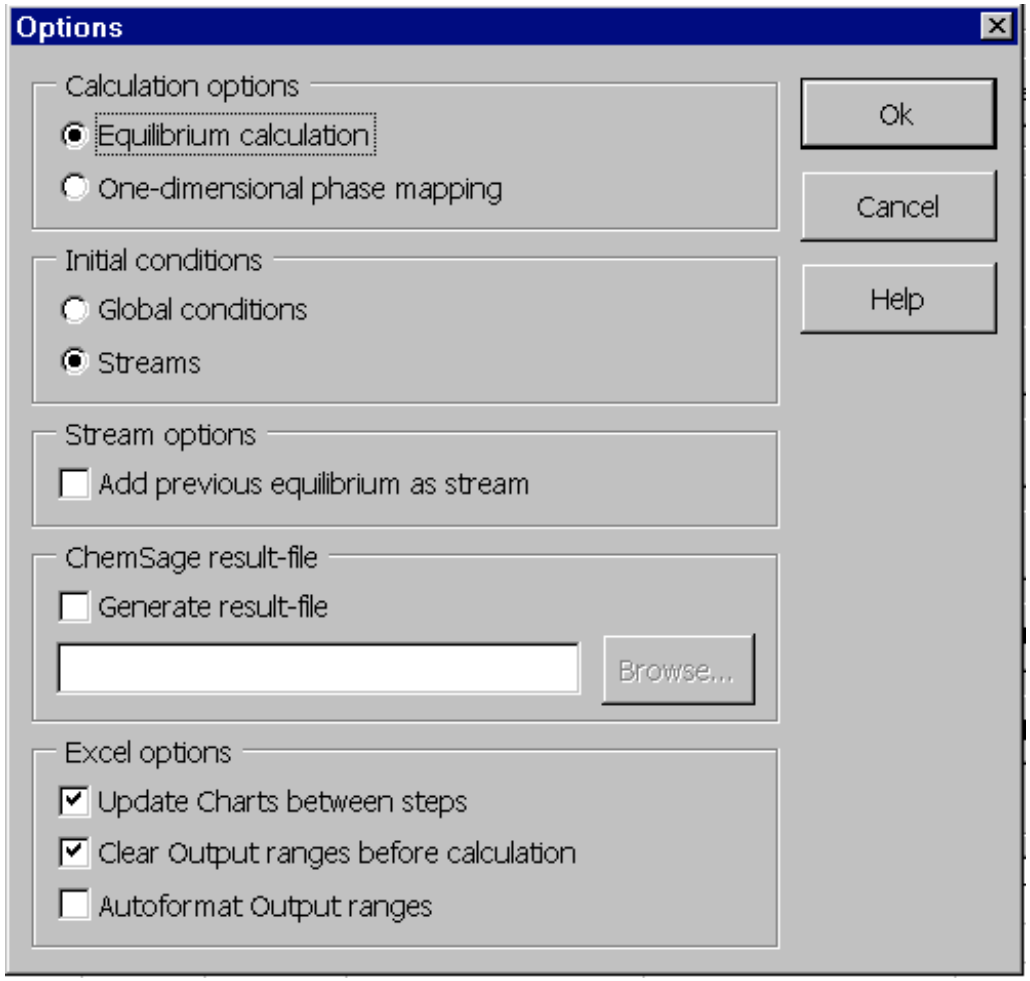
ChemSheet Example – Precipitation of Carbon



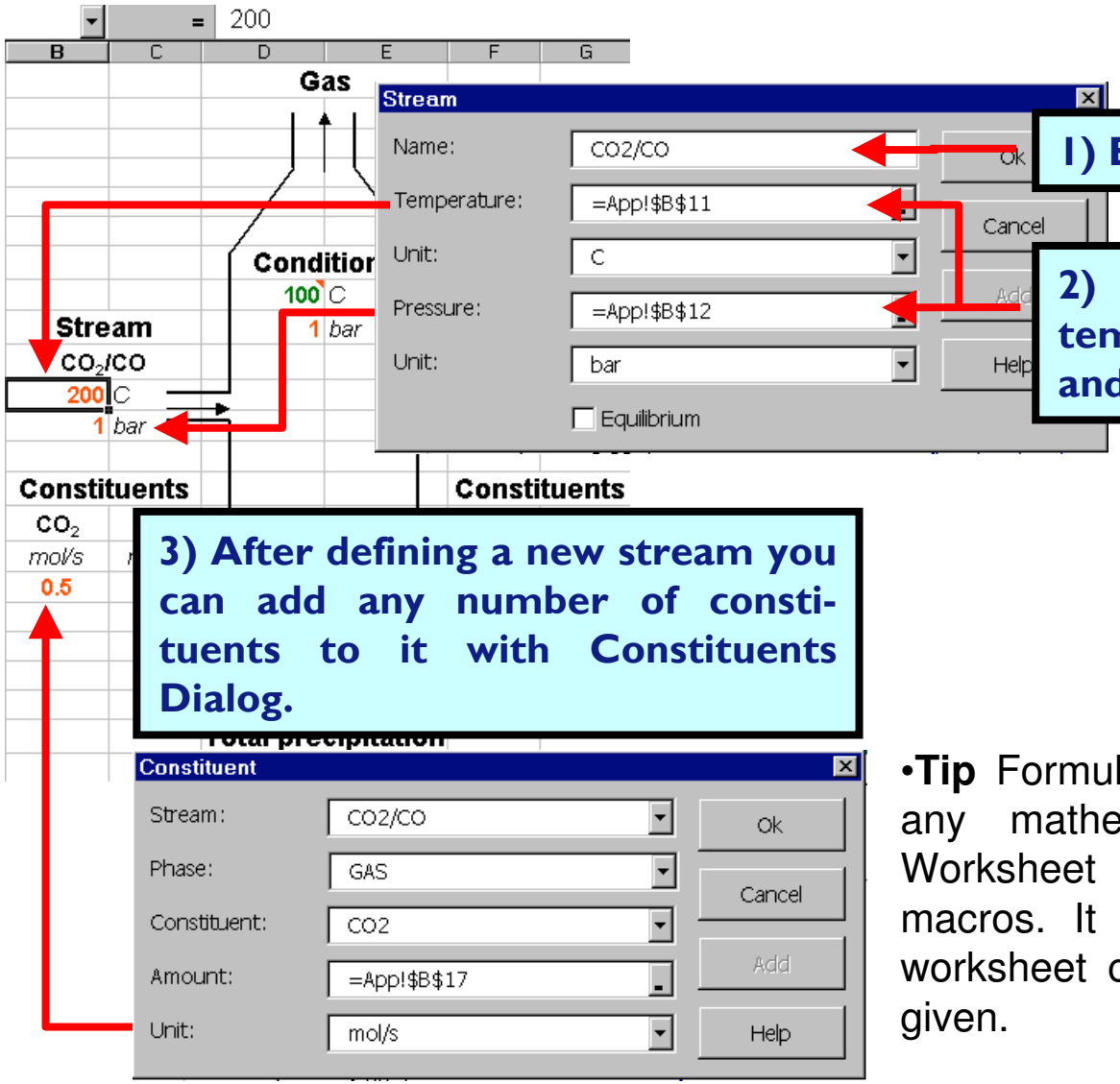
ChemSheet Dialog



Options Dialog



Defining Streams



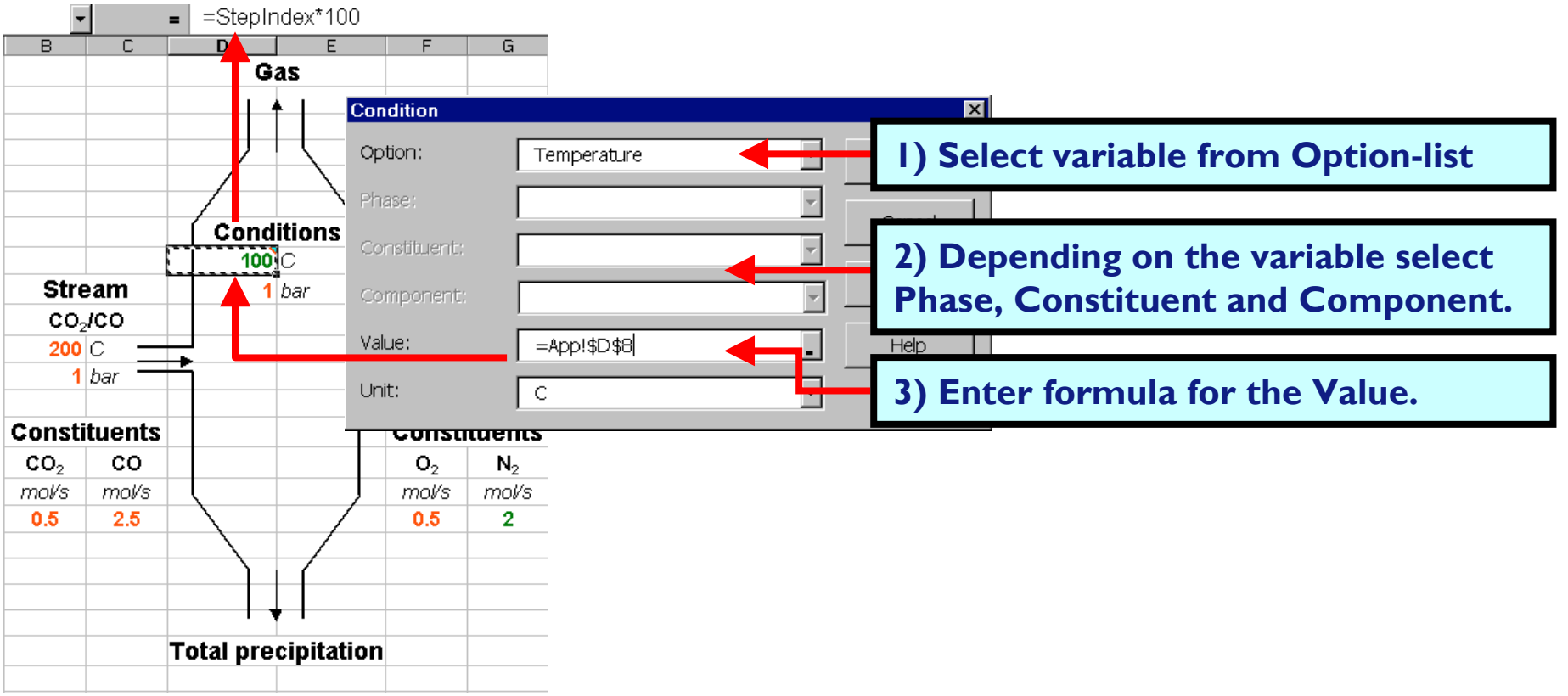
1) Enter name for the stream

2) Enter formulas for the temperature and pressure and their units.

3) After defining a new stream you can add any number of constituents to it with Constituents Dialog.

•**Tip** Formula can be a constant, contain any mathematical operations or any Worksheet functions or user-defined macros. It can also be a reference to worksheet cell where the actual value is given.

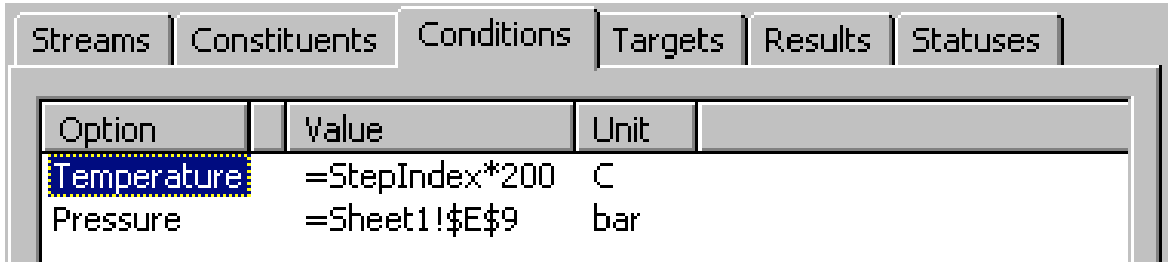
Defining Streams



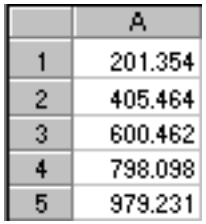
•**Tip** It is easier to change the value later if it is given in a worksheet cell. So it is advised to place those values directly on worksheet and other values could be “hidden” inside ChemSheet.

Using Formulas

•Enter formula that uses StepIndex and some scaling value (here 200).
Use this method if the value changes gradually.



•Enter Excel worksheet function INDEX that uses Worksheet Range and StepIndex.
Use this method if the temperature changes in way that is not easy to formulate.



•**Tip** Instead of worksheet functions you can also use your own macros. Just remember to pass **StepIndex** to it as a variable so it is called automatically every time when **StepIndex** changes.

```
Function MyFun(StepIndex as Variant) as Variant
   MyFun = StepIndex
End Function
```

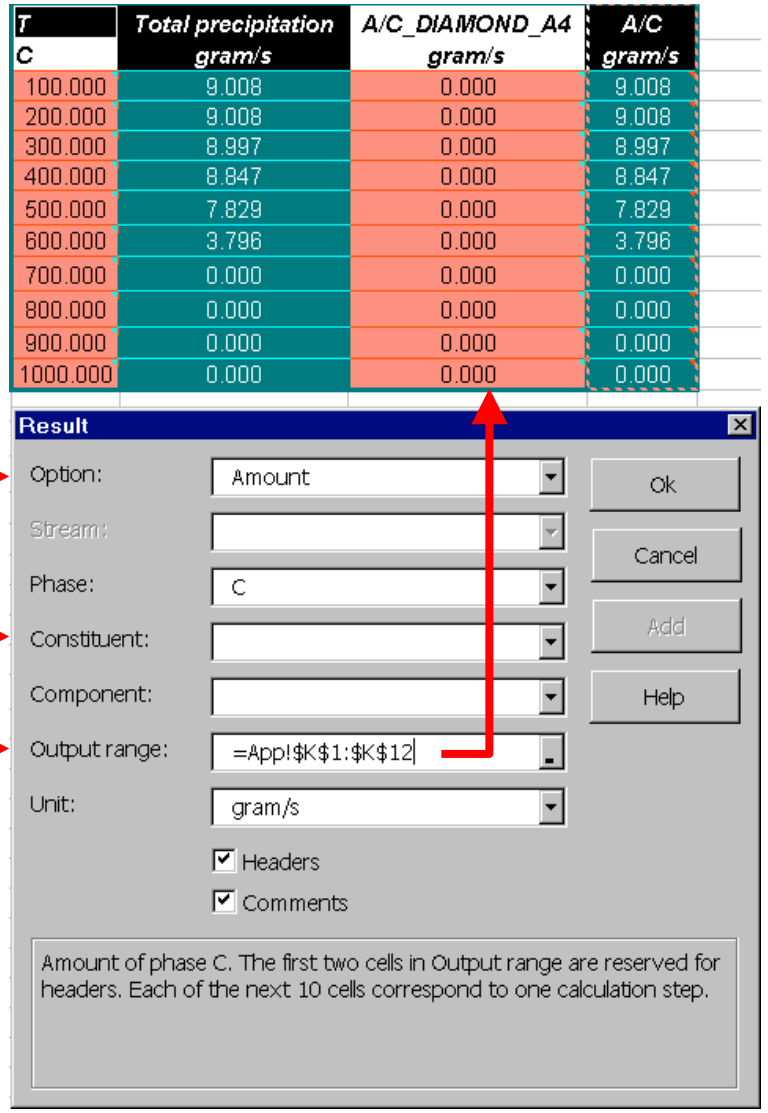
An example macro macro that returns StepIndex

Using Formulas

1) Select variable from Option-list

2) Depending on the variable select Phase, Constituent and Component.

3) Select Output range on worksheet where to store the values for the selected variable.
NOTE Remember to include enough cells for all calculation steps.



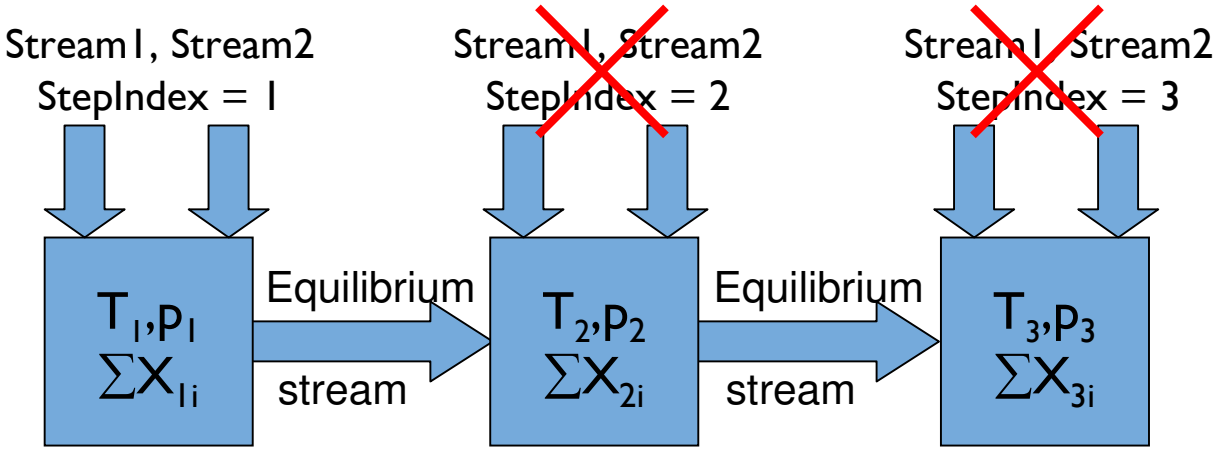
•**Tip** Using ***ALL*** as **Phase**, **Constituent** or **Component** name you can output many values at once.

NOTE Remember to include enough columns in **Output range** for all the values as each value is stored to separate column.

Advanced Options

•Normally the successive calculation steps are not connected with each other.

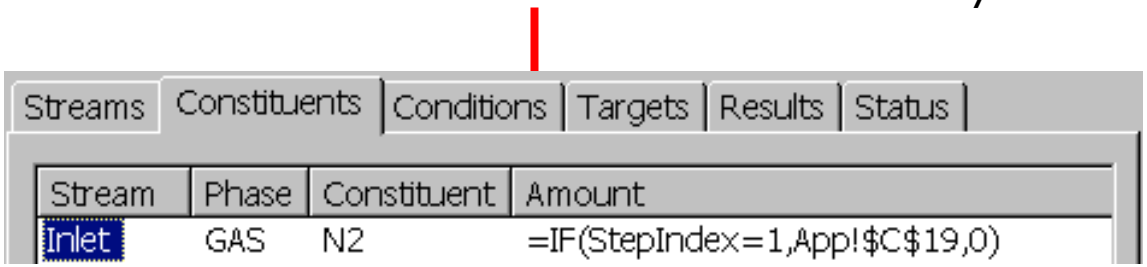
•You can connect successive calculations steps by using "**Add previous equilibrium as stream"**-option. The results from previous equilibrium are added automatically to the next calculation.



Schematic example of a model with three steps and two streams. When using "Add previous equilibrium as stream"-option the streams should be inputted only to the first "step". Then the results from the first step are automatically added to subsequent steps.

•**NOTE** You have to make sure <u>not</u> to add streams for each calculation step as then they would be added more than once. You should activate the constituents for each stream only at that step in which they should be inputted.

See the Pipe.xls example in \Samples directory and the next slide



Stack Gas Option

Streams | Constituents | Conditions | Targets | Results | Status

Option	Phase	Value	Unit
Enthalpy		=App!$C$28	J/s
Pressure		=1	bar

Streams | Constituents | Conditions | Targets | Results | Status

Option		Initial...	Lower ...	Upper limit	Unit
Tempe...		=1000	=298.15	=6000	K

Streams | Constituents | Conditions | Targets | Results | Status

Stre...	Ph...	Co...	Amount
Inlet	GAS	N2	=IF(StepIndex=1,App!$C$19,0)
Inlet	GAS	O2	=IF(StepIndex=1,App!$C$20,0)
Inlet	GAS	CO2	=IF(StepIndex=1,App!$C$21,0)
Inlet	GAS	CO	=IF(StepIndex=1,App!$C$22,0)
Air	GAS	N2	=IF(StepIndex=INT(StepCount/2),App!$C$13,0)
Air	GAS	O2	=IF(StepIndex=INT(StepCount/2),App!$C$14,0)

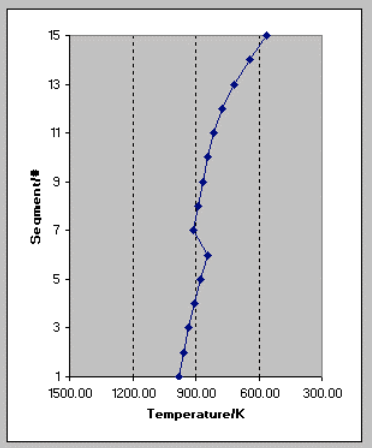
C28 = =3.14*do*h*(298.15-IF(StepIndex=1,C17,INDEX(T,StepIndex-1,1)))/(do/(hi*di)+do*LOG(do/di)/(2*lw)+1/ho)

Pipe dimensions		
r diameter	0.3	m
er diameter	0.35	m
ss-sectional area	0.07065	m2
l height	15	m
ht of segment	1	m
of segment	0.942	m2

Air feed		
perature	298.15	K
sure	1	bar
/N2	1.5	mol/s
/O2	0.375	mol/s

Inlet feed		
Temperature	1000	K
Pressure	1	bar
GAS/N2	0.5	mol/s
GAS/O2	0.125	mol/s
GAS/CO2	0.5	mol/s
GAS/CO	2.5	mol/s

Heat transfer		
Inner wall coeff.	500	W/m2-K
Outer wall coeff.	50	W/m2-K
Thermal conductivity	5	W/m-K
Heat transfer	-31258	W



Segment #	T K	H J/s	VT m3/s	Velocity m/s
1	977.54	-31258	0.27	3.80
2	955.52	-30257	0.25	3.53
3	932.80	-29277	0.23	3.28
4	908.14	-28265	0.21	3.04
5	879.92	-27167	0.20	2.80
6	845.42	-25910	0.18	2.57
7	910.48	-24373	0.37	5.28
8	890.52	-27271	0.35	5.02
9	868.32	-26382	0.34	4.76
10	842.67	-25393	0.32	4.50
11	811.57	-24251	0.30	4.23
12	771.44	-22866	0.28	3.95
13	716.15	-21078	0.26	3.61
14	641.50	-18616	0.23	3.21
15	561.71	-15292	0.20	2.81

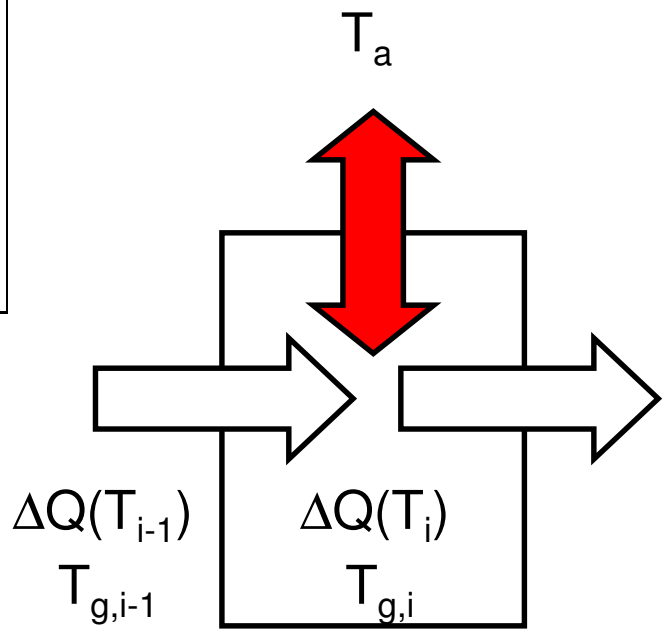
$$Q = \frac{\pi \cdot d_o \cdot h \cdot (T_a - T_g)}{\frac{d_o}{h_i \cdot d_i} + \frac{d_o}{2 \cdot \lambda_w} \ln \frac{d_o}{d_i} + \frac{1}{h_o}}$$

This example uses temperature as a target variable. Enthalpy change for each step is calculated using heat transfer from gas to ambient air through pipe wall. Gas cools down as it exchanges heat with the surroundings. At the middle of the pipe an additional air feed is introduced.

Heat Transfer = Enthalpy Change

•From heat transfer equation we get the enthalpy condition for calculation

$$Q = \frac{\pi \cdot d_o \cdot h \cdot \left(T_a - T_g\right)}{\frac{d_o}{h_i \cdot d_i} + \frac{d_o}{2 \cdot \lambda_w} \ln \frac{d_o}{d_i} + \frac{1}{h_o}}$$



•Heat transfer is function of unknown temperature (result from of next calculation).

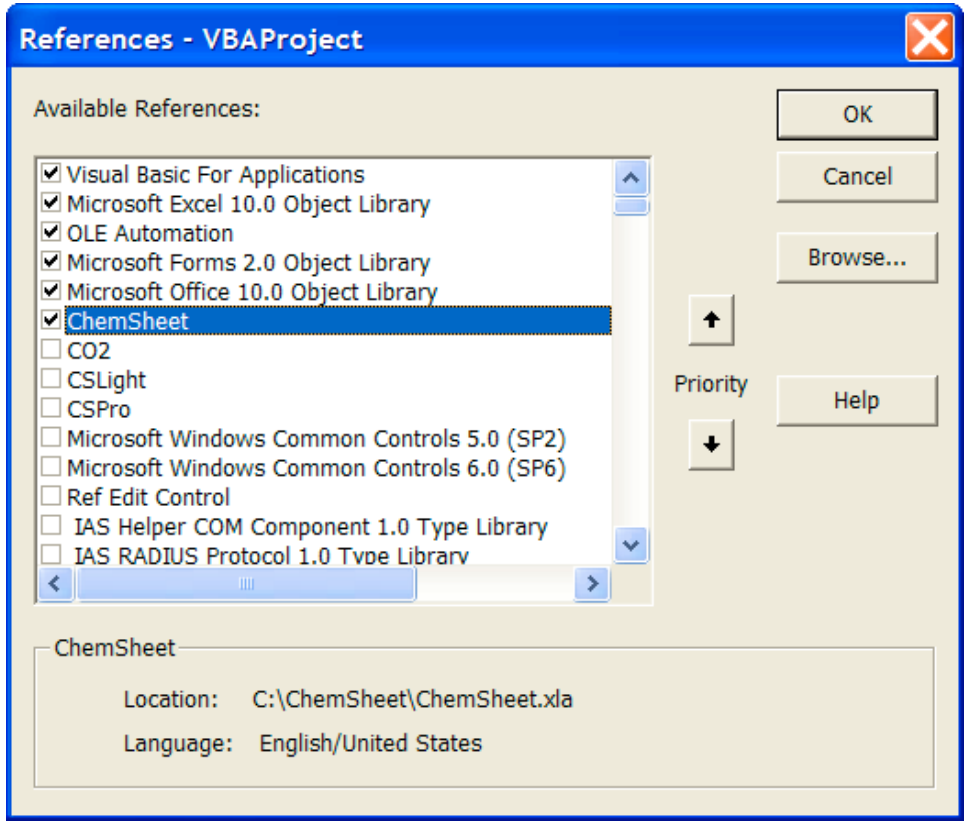
•Approximation is to use temperature from previous calculation.

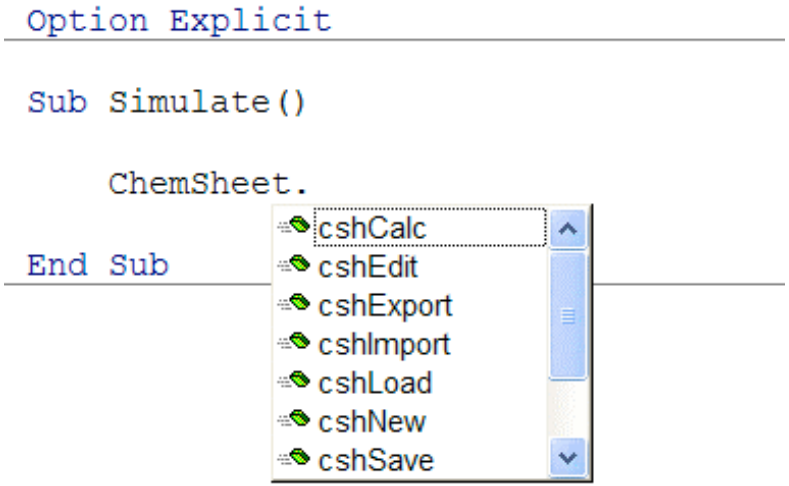
•Only one iteration is required

$\Delta Q(T_{i-1}) \Rightarrow T_{g,i}$

Using ChemSheet in VBA

- Add reference to ChemSheet add-in





- cshCalc
- cshExport Range
- cshImport Range

ChemSheet Examples:

Deep Impact - Asteriod Collision with Earth

Copper Sulphide Flash Smelting

Methane Reformer in SOFC Process (exhibits kinetic inhibitions)

Scheil Cooling Sequence of a Binary Alloys

ChemSheet Example: Deep Impact

- What happens if asteroid **500 km** in diam. collides with the earth?

Deep Impact: Step By Step

Asteroid enters the upper atmosphere at a speed of between 11 and 72 km/s on a trajectory between normal incidence (90 °) and a grazing impact, parallel to the Earth's surface (0 °).

The abrupt deceleration of asteroid as it collides with the Earth transfers kinetic energy from the asteroid to the target. As a result, the target and impactor are compressed to huge pressures and heated to enormous temperatures.

In the wake of the expanding shock wave, the target is comprehensively fractured, shock-heated, shaken, and set in motion—leading to the excavation of a cavity many times larger than the impactor itself. This temporary cavity (often termed the transient crater) subsequently collapses under the influence of gravity to produce the final crater form[1].

The kinetic energy of the impactor is ultimately converted into thermal energy, seismic energy, and kinetic energy of the target and atmosphere. The increase in thermal energy melts and vaporizes the impactor and some of the target rocks[1].

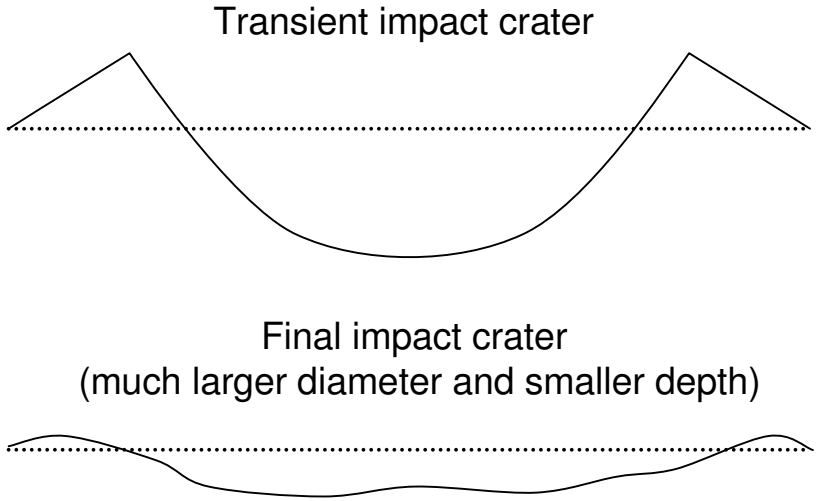
[1]G. S. Collins ,H. J. Melosh and R. A. Marcus: in Meteoritics & Planetary Science 40, Nr 6, 817–840 (2005)

Deep Impact: Asteroid Energy

- Kinetic energy of asteroid:

$$E = \frac{1}{2} m v^2$$

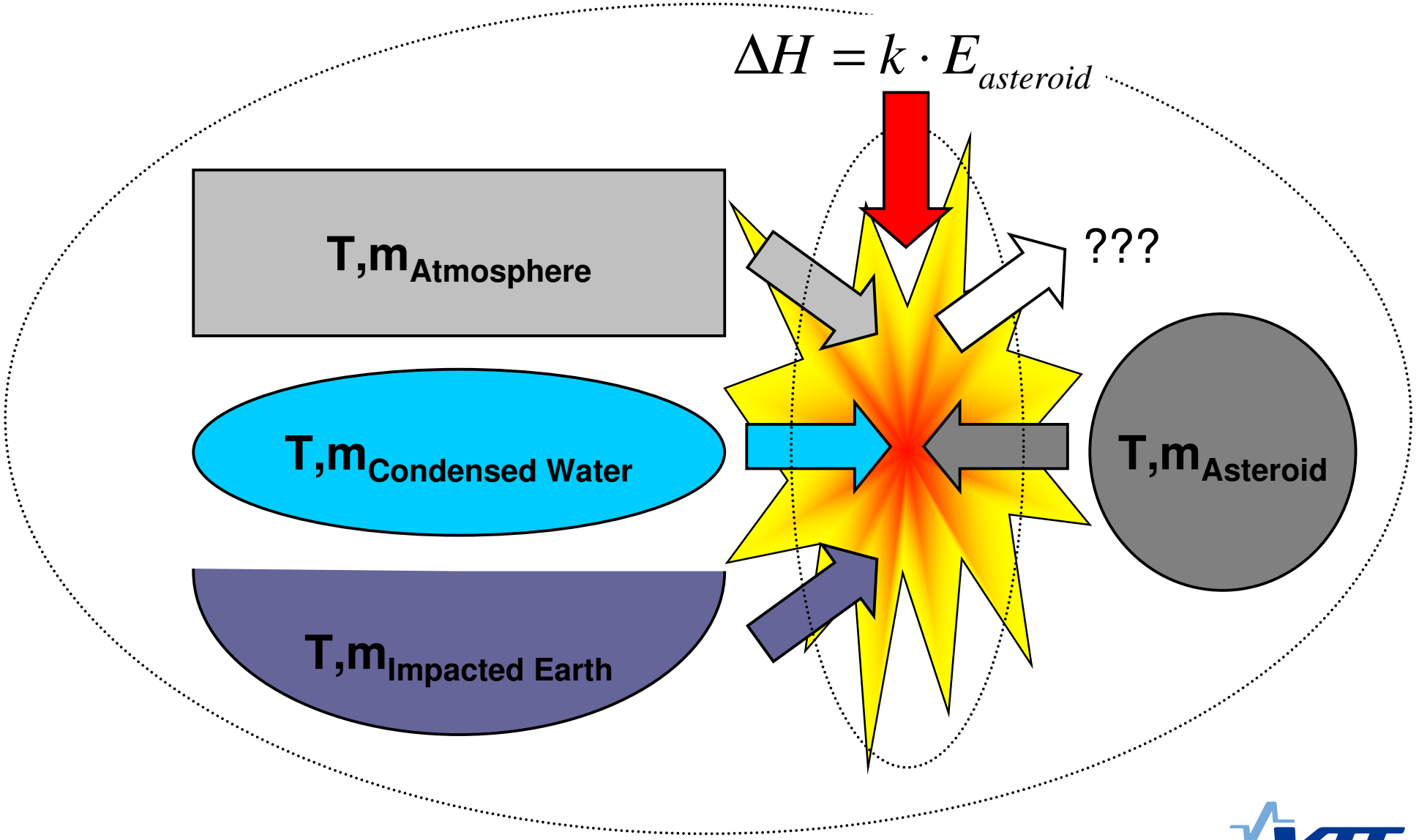
- Kinetic energy of asteroid is converted to:
  - thermal heat
  - seismic waves (~1E-4 of E_{kin})
  - blast waves
  - sound waves
  - flying ejecta ...



➢ For those who are interested (online impact calculator):

http://www.lpl.arizona.edu/impacteffects

Deep Impact: Mass and Energy Balances



Deep Impact: Asteroid Composition

- Asteroid classes
  - Rocky
  - Metallic
- S-type rock asteroid
  - Typical mineral composition mixture of olivine and pyroxene
    - $MgSiO_3$ 66.7 mass-%
    - $FeSiO_3$ 33.3 mass-%

➢gives roughly correct elementary balance

➢Thermodynamic data available in FactSage

✓Gas	ideal solution
✓Slag(l)	non-ideal solution
✓Orthopyroxene(s)	non-ideal solution
✓Olivine(s)	non-ideal solution
✓Condensed phases(s)	pure solids

➢Equilibrium composition ~ orthopyroxene

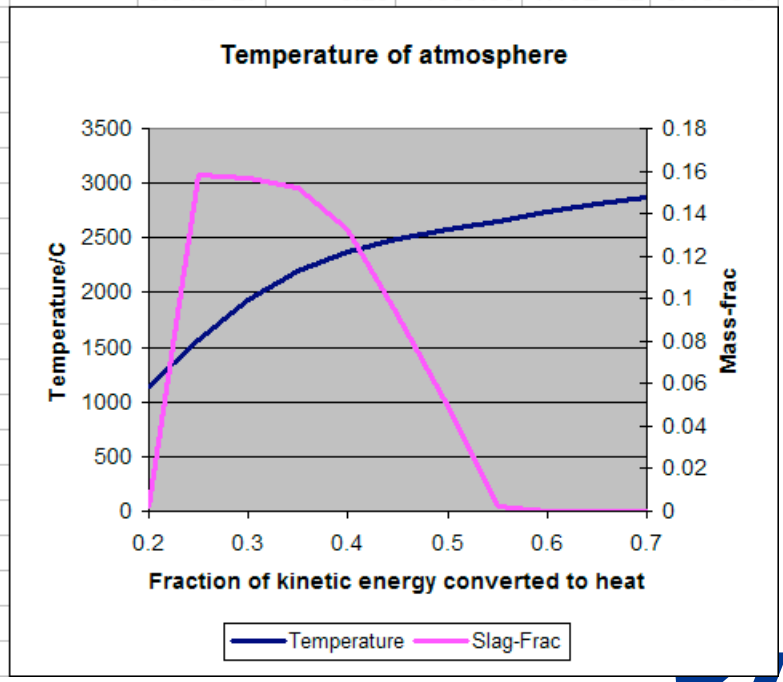
Deep Impact: ChemSheet Model

Rock asteroid					
Temperature	-100	C			
Density	2700	kg/m3			
Diameter	500000	m			
Velocity	20000	m/s			
Volume	6.54E+16	m3			
Mass	1.77E+20	kg			
MgSiO3	66.7	m-%	1.18E+20	kg	Rock asteroid
FeSiO3	33.3	m-%	5.88E+19	kg	
Condensed water					
Temperature	0	C			
Density	1000	kg/m3			
Volume	1.37E+09	km3			Estimation
H2O(Liq)	98.25	v-%	1.35E+21	kg	Salt ignored
H2O(Ice)	1.75	v-%	2.4E+19	kg	
Atmosphere					
Temperature	0	C			
Mass	5.15E+17	kg			Estimation
H2O	0.29	m-%	1.49E+15	kg	
N2	75.523	m-%	3.89E+17	kg	dry basis
O2	23.133	m-%	1.19E+17	kg	dry basis
Ar	1.288	m-%	6.63E+15	kg	dry basis
CO2	0.056	m-%	2.88E+14	kg	dry basis
Impacted earth					
Temperature	25	C			
Density	2700	kg/m3			
Volume	3.5E+08	km3			Estimation
Mass	9.45E+20	kg			
MgSiO3	33.3	m-%	3.15E+20	kg	
FeSiO3	66.7	m-%	6.3E+20	kg	

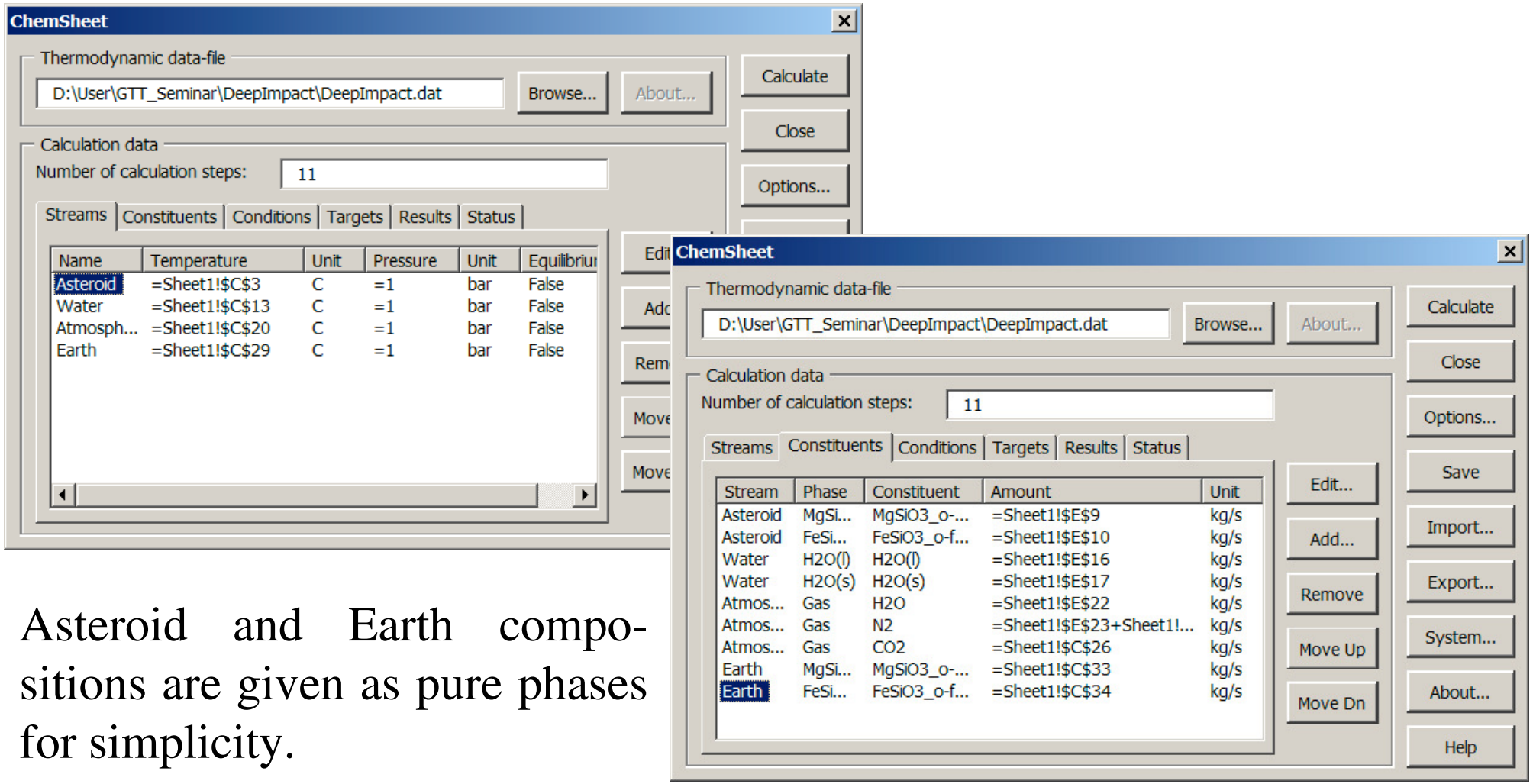
$$E = \frac{1}{2} m v^2$$

Combustion heat of TNT	4.18E+06	J/kg	
	4.18E+15	J/Mt	
Kinetic energy of asteroid	**3.53E+28**	**J**	
	8.45E+12	Megaton of TNT	
Fraction to thermal heat	**0.2**	Parameter	
Fraction to seismic energy	0.0001		
Magnitude = *0.67 log10 E - 2.9*	13.55	Richter scale	

	H	Hfrac	T	VT	Slag-Frac
	J/s	-	C	m3/s	-
	7.07E+27	0.2	1137.315	8.92E+21	0.002222
	8.84E+27	0.25	1559.96	1.16E+22	0.158094



Deep Impact: Stream Definitions



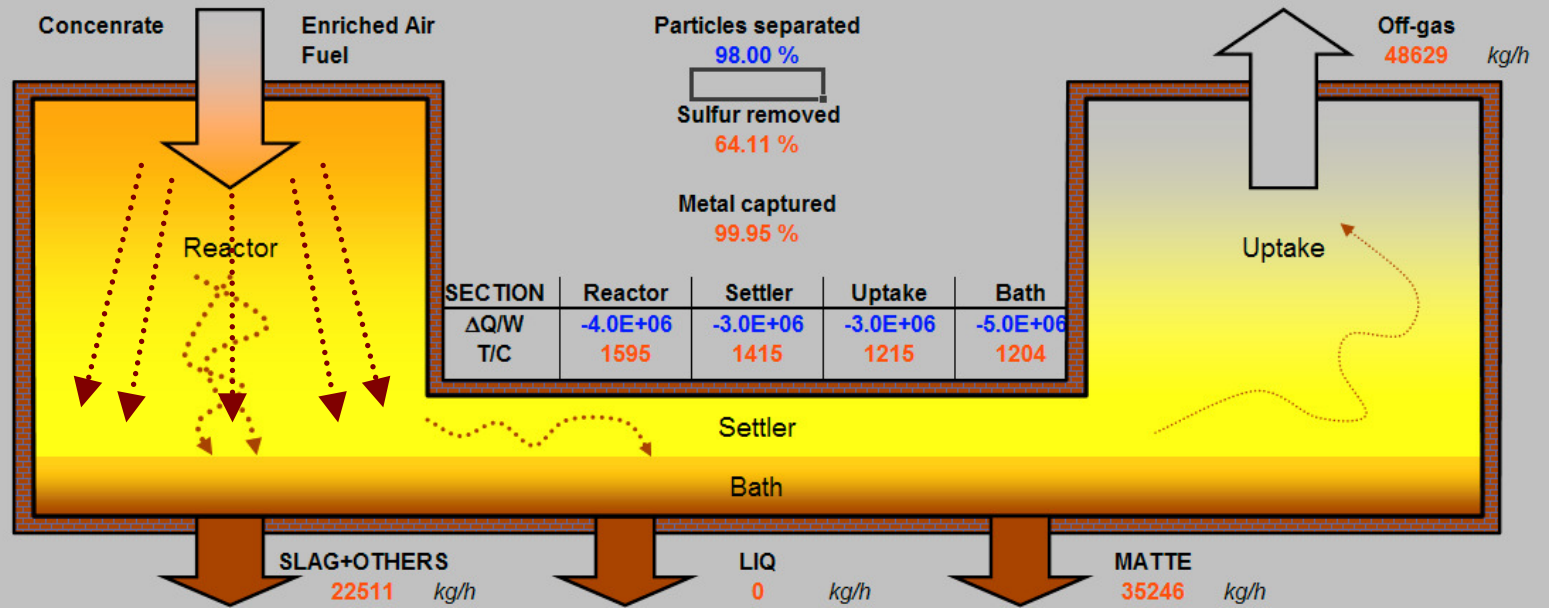
Asteroid and Earth compositions are given as pure phases for simplicity.

Copper Sulfide Flash Smelting

Concentrate				
Temp	60	C		
Pres	1	bar		
Flow	70000	kg/h		
Cu(s)	1	mass-%	700.000	kg/h
CuS(s)	16.8	mass-%	11760.000	kg/h
Cu2S(s)	0	mass-%	0.000	kg/h
CuFeS2(s)	41	mass-%	28700.000	kg/h
Cu5FeS4(s)	10	mass-%	7000.000	kg/h
FeS2(s)	22.4	mass-%	15680.000	kg/h
Fe2O3(s)	5	mass-%	3500.000	kg/h
SiO2(s)	3.1	mass-%	2170.000	kg/h
CaO(s)	0.1	mass-%	70.000	kg/h
Al2O3(s)	0.6	mass-%	420.000	kg/h
TOT	100	mass-%	70000.000	kg/h

Enriched Air				
Temp	40	C		
Pres	1	bar		
Flow	27000	nm3/h		
N2(g)	50	vol-%	16873	kg/h
O2(g)	50	vol-%	19273	kg/h
TOT	100	vol-%	36146	kg/h

Fuel				
Temp	60	C		
Pres	1	bar		
Flow	240	kg/h		
C8H10(l)	0	mass-%	0.000	kg/h
C8H18(l)	100	mass-%	240.000	kg/h
TOT	100	mass-%	240.000	kg/h



SECTION	Reactor	Settler	Uptake	Bath
ΔQ/W	-4.0E+06	-3.0E+06	-3.0E+06	-5.0E+06
T/C	1595	1415	1215	1204

Flash Smelting Process

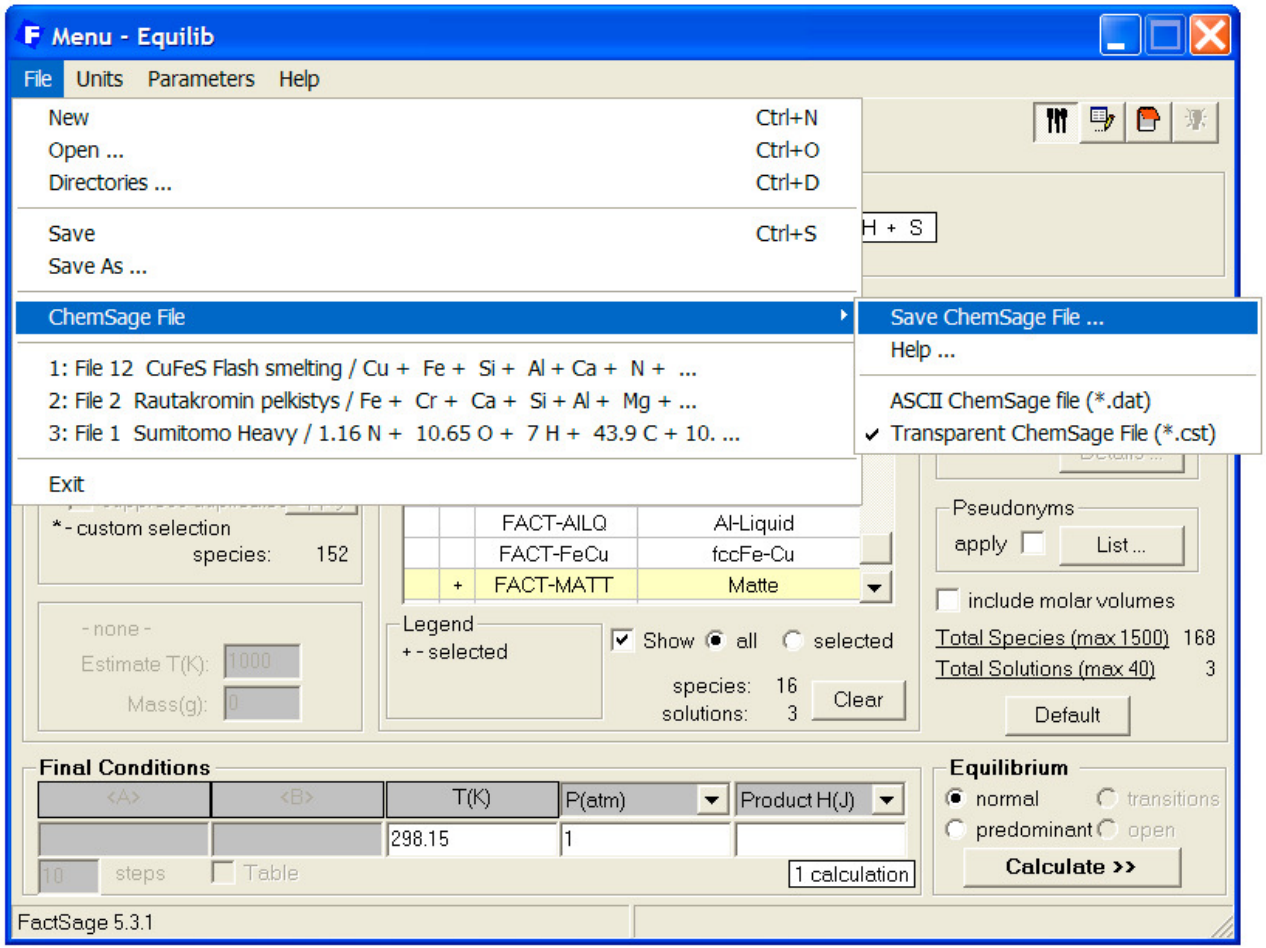
The copper ore (commonly chalcopyrite, $CuFeS_2$) is crushed and ground before it is concentrated to between 20 and 40% copper in a flotation process. The next major step in production uses pyrometallurgical processes to convert the copper concentrate to 99% pure copper suitable for electrochemical refining. These high temperature processes first smelt the concentrate in a furnace (**flash smelting**), then oxidise and reduce the molten products to progressively remove remaining sulfur, iron, silicon and oxygen to leave behind relatively pure copper.

The feed to flash smelting is known as copper **concentrate**. It contains copper and iron sulfides, silica and limestone grind to small particles (<100µm). **Flash smelting** is highly exothermic process. It requires almost no external heat. Concentrate and enriched air are fed to the **shaft** of the furnace. Iron oxides and sulfides are converted to liquid **slag**. Copper sulfides are first partly oxidized and then converted to liquid called **matte**. At the bottom of furnace slag and matte are collected as **bath** and separated from each other (lighter slag is floating on top of the heavier matte). The gas from furnace is mainly nitrogen and sulfur oxide.

Creating the Thermodynamic System

Thermodynamic data-file for copper sulfide flash smelting ChemSheet model was created with FactSage.

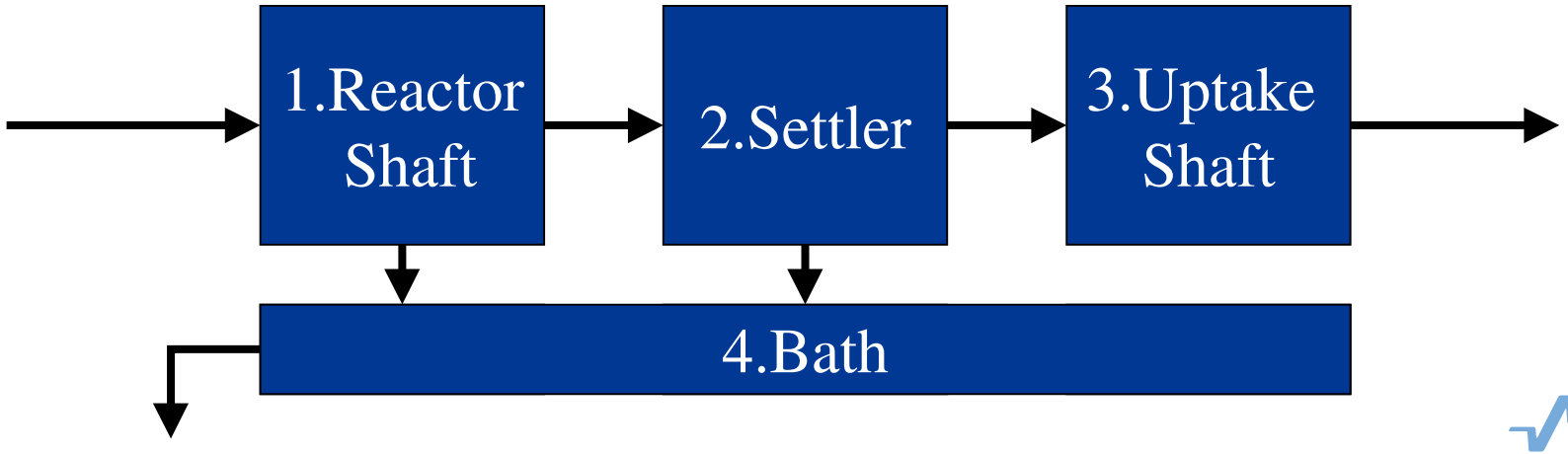
"The thermodynamic properties of the slag, matte, and liquid copper phases in the Cu-Ca-Fe-Si-O-S system have been critically assessed and optimized over the ranges of compositions of importance to copper smelting/converting based on thermodynamic and phase equilibria information available in the literature and using the modified quasichemical model."[1]



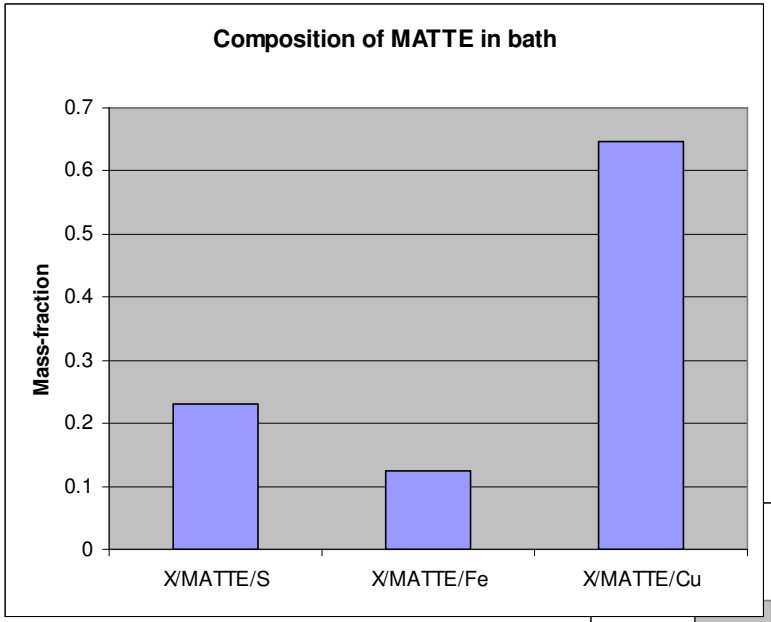
[1]A thermodynamic database for copper smelting and converting, Degterov, S., Pelton,A., METALLURGICAL AND MATERIALS TRANSACTIONS B, VOLUME 30B, AUGUST 1999

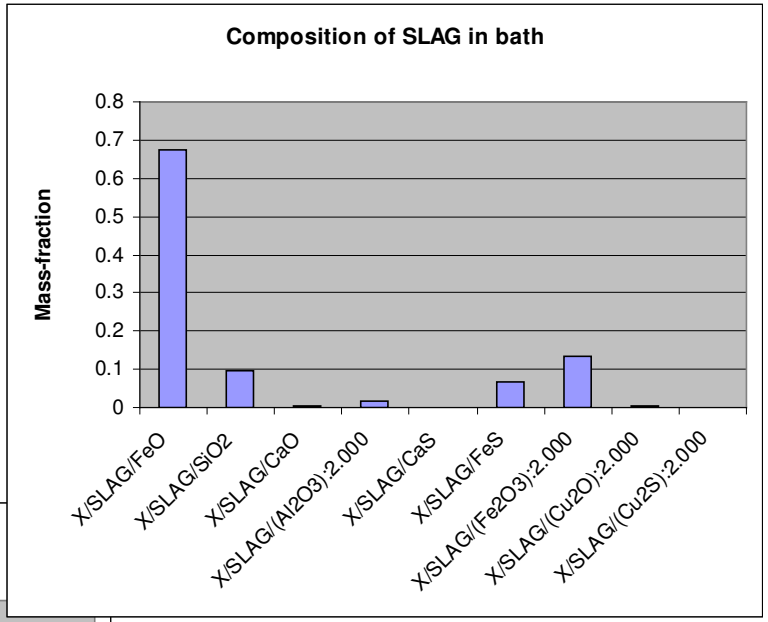
Flash Smelting Model

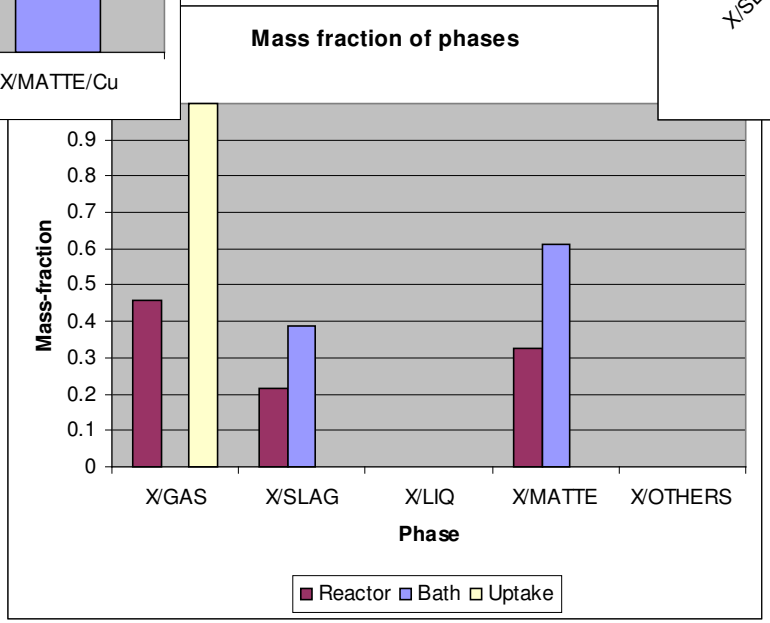
The flash smelting process is simulated with one ChemSheet model that contains four calculation steps. First step calculates flow temperature and composition in reactor shaft. The second step calculates flow temperature and composition is settler. Before going to settler solid and liquid phases are separated (using given separation efficiency) from gas as they are assumed to go to bath at the bottom of settler. The third step calculates flow temperature and composition in uptake shaft. Again remaining solid and liquid phases are separated (as gas temperature decreases it is possible that also condensation takes place) from gas. Fourth step calculates bath temperature and composition. Flows to bath consists of separated solids and liquids from reactor shaft and settler.



Flash Smelting Results

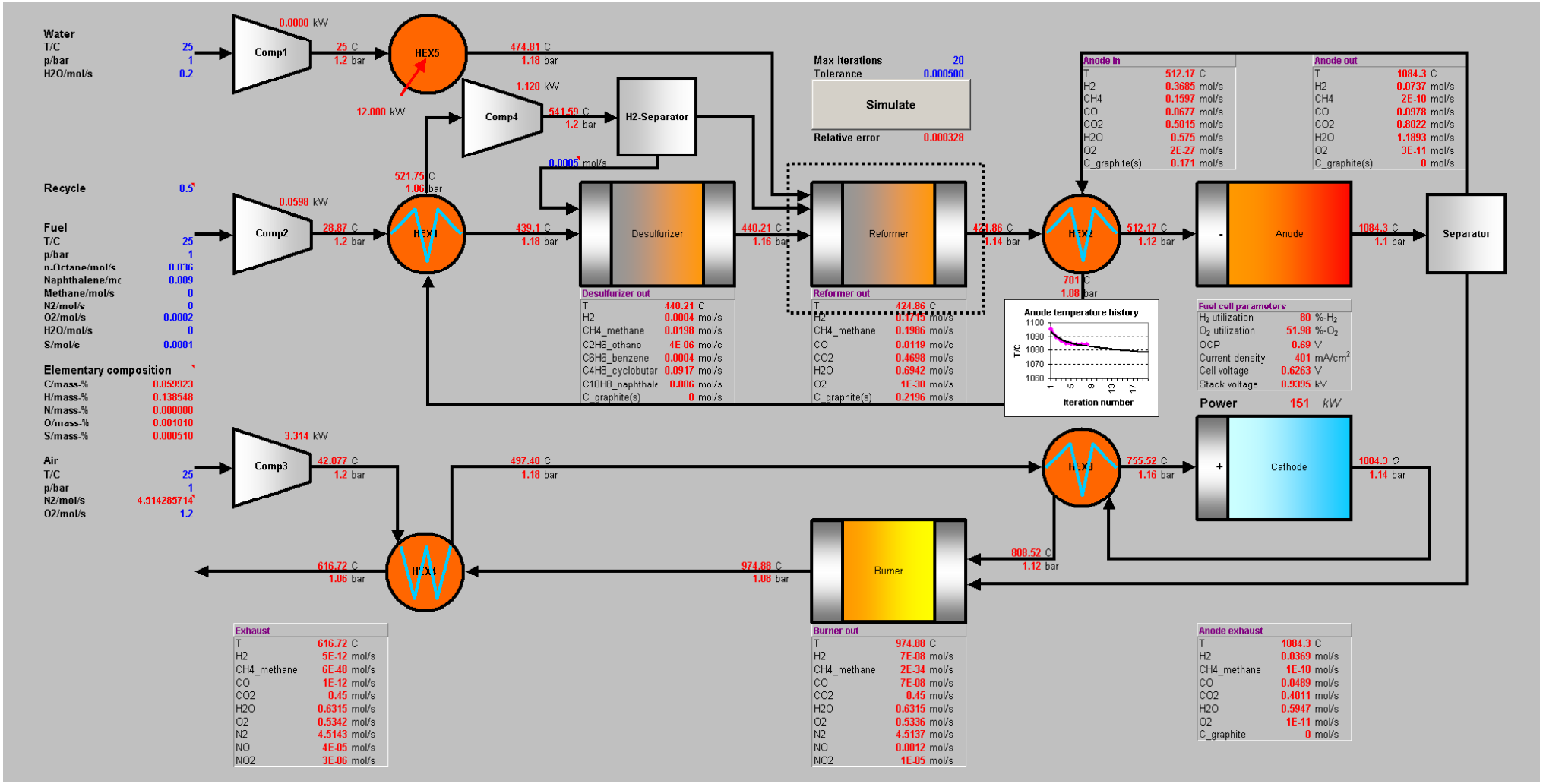






Methane Reformer in SOFC Process

Reformer unit operation in solid oxide fuel cell process



SOFC Reactions

The normal electrochemical reactions in solid oxide fuel cell:

Anode reactions	$CO(a)+O^{2-}$	$\rightarrow CO_2(a)+2e^-$
	$H_2(a)+O^{2-}$	$\rightarrow H_2O(a)+2e^-$
Cathode reaction	$O_2(c)+4e^-$	$\rightarrow 2O^{2-}$
Overall	$CO(a)+H_2(a)+O_2(c)$	$\rightarrow CO_2(a)+H_2O(a)$

Another way to represent the reactions is using only the oxygen:

Anode reaction	$2O^{2-}$	$\rightarrow O_2(a)+4e^-$
Cathode reaction	$O_2(c)+4e^-$	$\rightarrow 2O^{2-}$
Overall	$O_2(c)$	$\rightarrow O_2(a)$

Cell Potential

Gibbs energy change for the overall reaction is given as:

$$\Delta G = \Delta G^0 + RT \ln \frac{a_{O_2}(a)}{a_{O_2}(c)}$$

$$\Delta G^0 = 0$$

$$-nFE_{rev} = \Delta G$$

The reversible cell potential, E_{rev}, can be given as:

$$E_{rev} = \frac{RT}{4F} \ln \frac{a_{O_2}(c)}{a_{O_2}(a)}$$

Or using normal representation (see previous slide):

$$E_{rev} = E^0_{H_2} - \frac{RT}{2F} \ln \frac{p_{H_2O}}{p_{H_2}\left(p_{O_2}\right)^{1/2}}$$

Reformer

Makeup steam and optional recirculeted anode products (containing steam) are fed to the reformer with fuel (methane and other hydrocarbons). Methane and steam react together in reformer to produce reactants to anode.

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2$$

The reaction happens in elevated temperatures and in the present of nickel based catalyst in tubular packed bed. Also other reactions take places. The most probable is the shift reaction:

$$CO + H_2O \Leftrightarrow CO_2 + H_2$$

Carbon may also be present as longer chains than methane (depending on the composition of fuel). The reaction mechanisms in fuel may be very complex and may contain several hundreds of species. In order to simplify things only the time-dependent reaction of methane in considered. The reaction in the reformer can be given as follows :

$$r = k_0 e^{\frac{-Ea}{RT}} p_{CH_4}^n m_{cat}$$

Restricted Thermodynamic System

•Equilibrium and kinetics can be combined by introducing additional mass balance constrains

SOFC Thermodynamic system							
Phase	Constituent	Components					Restriction
		C	H	N	O	S	C*
Gas	H		1				
	H2		2				
	CH3_methyl	1	3				1
	CH4_methane	1	4				1
	....	...	...	...	...	...	...
	C8H18_octane	8	18				8
	C10H8_naphthalene	10	8				10
	...	...	...	...	...	...	...
	N2			2			
	O2				2		
	H2O		2		1		
	CO		1		1		
	CO2		1		2		
	...	...	...	...	...	...	...
	S					1	
	H2S		1			1	
Liquids	H2O(l)		2		1		
	...	...	...	...	...	...	...
Solids	C_graphite(s)	1					
	S_orthorhombic(s)					1	
Restrictions	C+						1
	C-						-1

Using Restrictions 1

For example the initial composition of system is 1 mol “C8H18_octane(l)” at 273.15 K and 1 bar. When equilibrium is calculated so that the system is allowed to go to equilibrium between all species (status of “C+” and “C-“ phases is “ENTERED” and their input values are 0) the following results are obtained

CH4_methane:	4.50
C_graphite:	3.50
C+:	3.50

It can be seen that “C_graphite” and equal amount of “C+” species is formed. That is because C8H18 contains 8 mol of “C*” component and also stoichiometry of “C+” contains the same component. So in equilibrium calculation C8H18 can react to CH4_methane and C_graphite because “C*” component is allowed to go to “C+”.

When same equilibrium is calculated so that the system is not allowed to go to equilibrium between all species (status of “C+” and “C-“ phases is “ELIMINATED”) the following results are obtained.

CH4_methane:	1.00
C4H8_cyclobutane:	1.75

This time no “C_graphite” is formed because status of “C+” is “ELIMINATED”. That means that equilibrium of “C8H18_octane(l)” is calculated only between those species that contain “C*” component and are not “ELIMINATED” from the calculation.

Using Restrictions 2

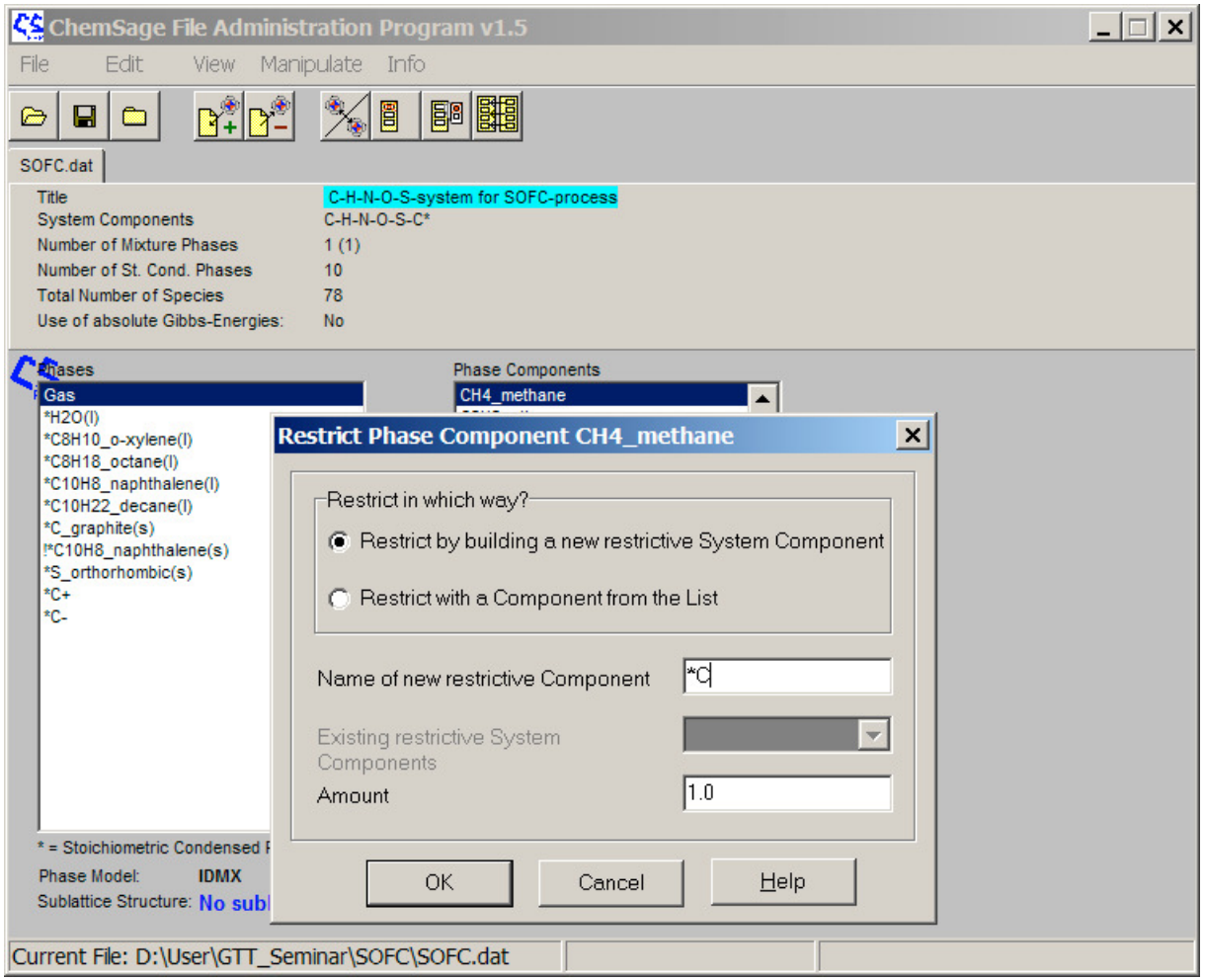
In the last example the same equilibrium is calculated so that 0.25 mol of “C8H18_octane(l)” is allowed to go to equilibrium between all species (status of “C+” is “ELIMINATED” and status of “C-“ is “ENTERED” and its initial amount is 2 mol (= 25 % of “C*” in “C8H18_octane”)) the following results are obtained.

CH4_methane:	3.00
C4H8_cyclobutane:	0.75
C_graphite:	2.00
C+:	0.00

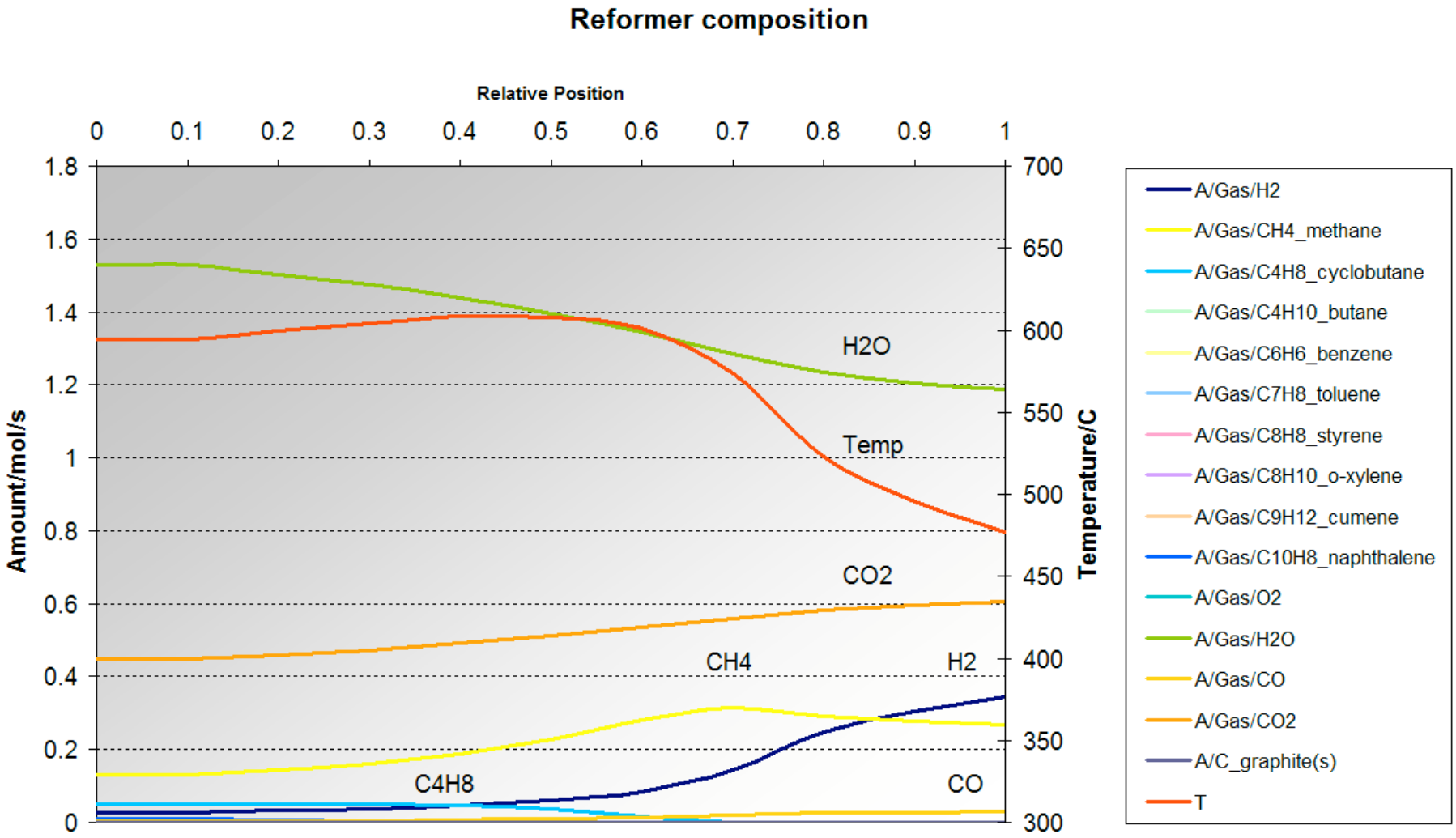
So in this case 2 mole of “C_graphite” is formed. This is possible because in input the amount of “C*” was 8 mol - 2 mol = 6 mol (from input values and stoichiometries of “C8H18_octance(l)” and “C-“). So at equilibrium the amount of “C*” is still 3 mol + 3 mol = 6 mol (“CH4_methane” and “C4H8_cyclobutane”)

Adding Restrictions

- Ascii datafiles can be edited by hand (= easy to make mistakes)
- CSFAP (from GTT) can be used to edit datafiles and also add restrictions



Calculated Reformer Composition



High CO_2 comes from recirculated anode reactants

”Calphad” Scheil Solidification

•System Pb-Sn, phases Liquid/BCT/FCC

•Initial Composition (1)
Pb 80 at-%
Sn 20 at-%

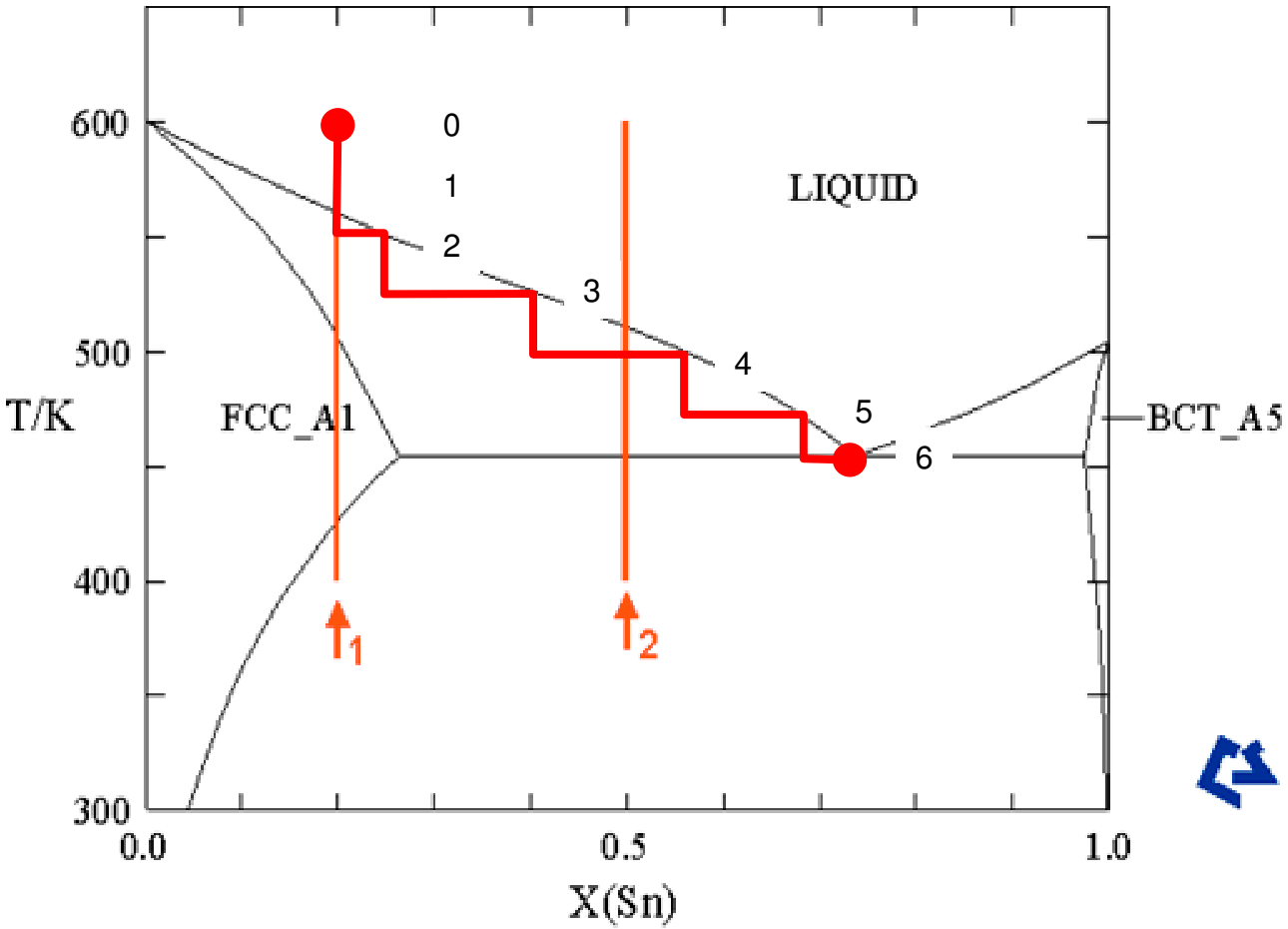
•Initial Temperature
600 K
•Temperature step
25 K (in the picture)

•Equilibrium calculation at each temperature step

•Formed solids removed

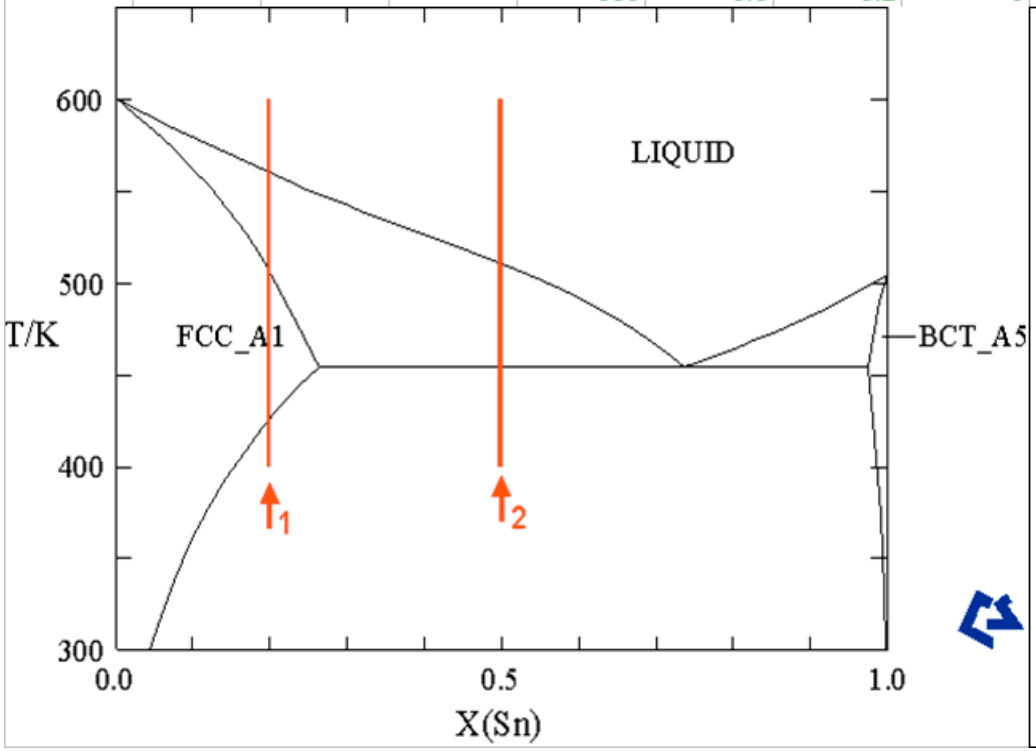
•Only remaining liquid goes to the next equilibrium calculation

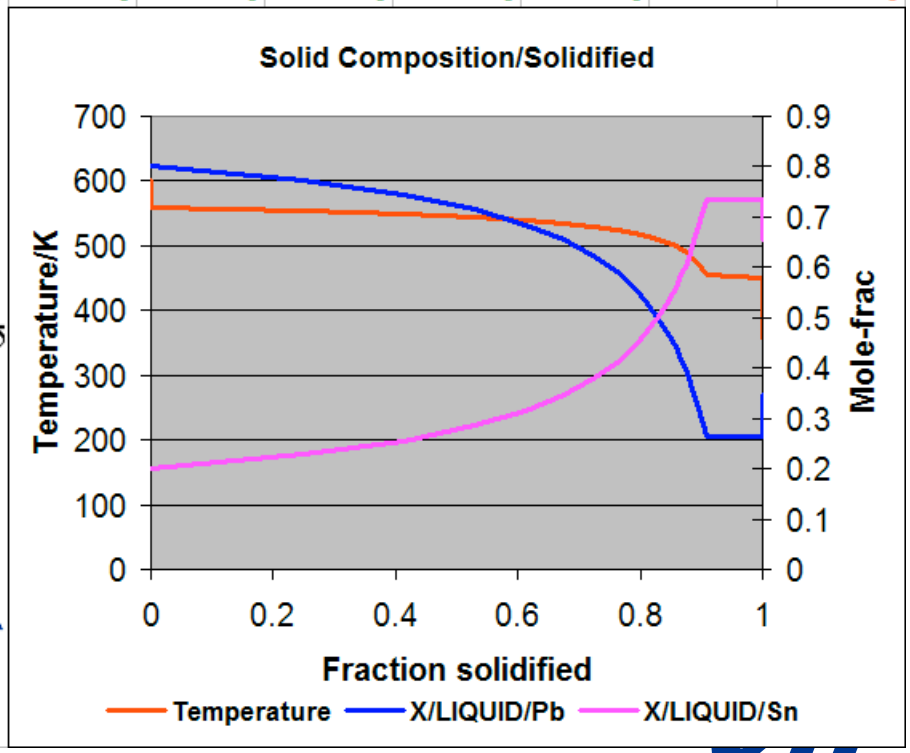
➢Liquid composition approaches eutectic



ChemSheet Scheil Solidification

Initial				T	A/LIQUID/	A/LIQUID/	A/BCT_A5	A/BCT_A5	A/BCT_A5	A/BCT_A5	A/FCC_A1	A/FCC_A1/Sn		A/Pb
T	600	K		K	mol	mol	mol	mol	mol	mol	mol	mol		mol
P	1	bar		355	0	0	0.000448	0.065429	0	0	0.023893	0.002461		0.024341
Pb0	0.8	mol												
Sn0	0.2	mol												Accumulat
				T	A/LIQUID/	A/LIQUID/	A/BCT_A5	A/BCT_A5	A/BCT_A5	A/BCT_A5	A/FCC_A1	A/FCC_A1/Sn		A/BCT_A5
Next				K	mol	mol	mol	mol	mol	mol	mol	mol		mol
Pb	0.8	mol		600	0.8	0.2	0	0	0	0	0	0		0
Sn	0.2	mol		595	0.8	0.2	0	0	0	0	0	0		0
DT	5			590	0.8	0.2	0	0	0	0	0	0		0
T	600			585	0.8	0.2	0	0	0	0	0	0		0
				580	0.8	0.2	0	0	0	0	0	0		0





Using Formulas and Results

•Simple Excel formulas and ChemSheet results are used to set incoming liquid

•Result in G4 contains amount of liquid Pb from last equilibrium and result in P4 contains total amount of Pb (used if all liquid is solidified).

MOD =IF(StepIndex=1,C5,IF(G4>0,G4,P4))

	A	B	C	D	E	F	G	H
1								
2		Initial				T	A/LIQUID/	A/LIQUID/
3		T	600	K		K	mol	mol
4		P	1	bar		355	0	0
5		Pb0	0.8	mol				
6		Sn0	0.2	mol				
7						T	A/LIQUID/	A/LIQUID/
8		Next				K	mol	mol
9		Pb	=IF(StepIr	mol		600	0.8	0.2
10		Sn	0.2	mol		595	0.8	0.2
11		DT	5			590	0.8	0.2
12		T	600			585	0.8	0.2
13						580	0.8	0.2

Condition

Option:	Incoming amount
Phase:	LIQUID
Constituent:	Pb
Component:	
Value:	=Sheet1!$C$9
Unit:	mol

Ok / Cancel / Add / Help

Result

Option:	Amount
Stream:	
Phase:	ALL
Constituent:	ALL
Component:	
Output range:	=Sheet1!$G$2:$N$4
Unit:	mol

Ok / Cancel / Add / Help

☑ Headers

☐ Comments

Amounts for all constituents (8) in all phases (4). The first two rows in Output range are reserved for headers. Each of the next 50 rows correspond to one calculation step and each column correspond to one constituent in one phase.