9th GTT Technologies Work Shop

Some Industrial Applications of FactSage and its family products in UBE Industries, LTD

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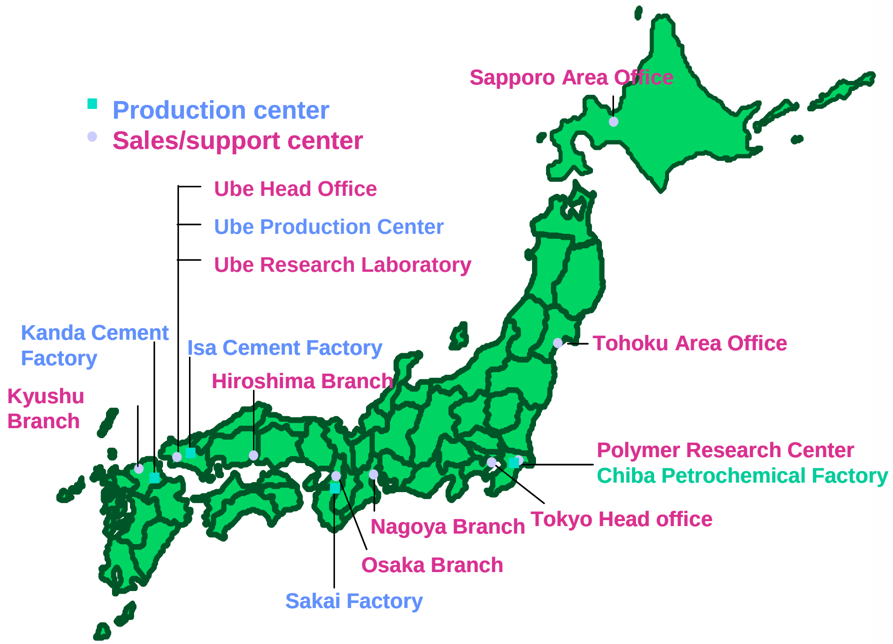
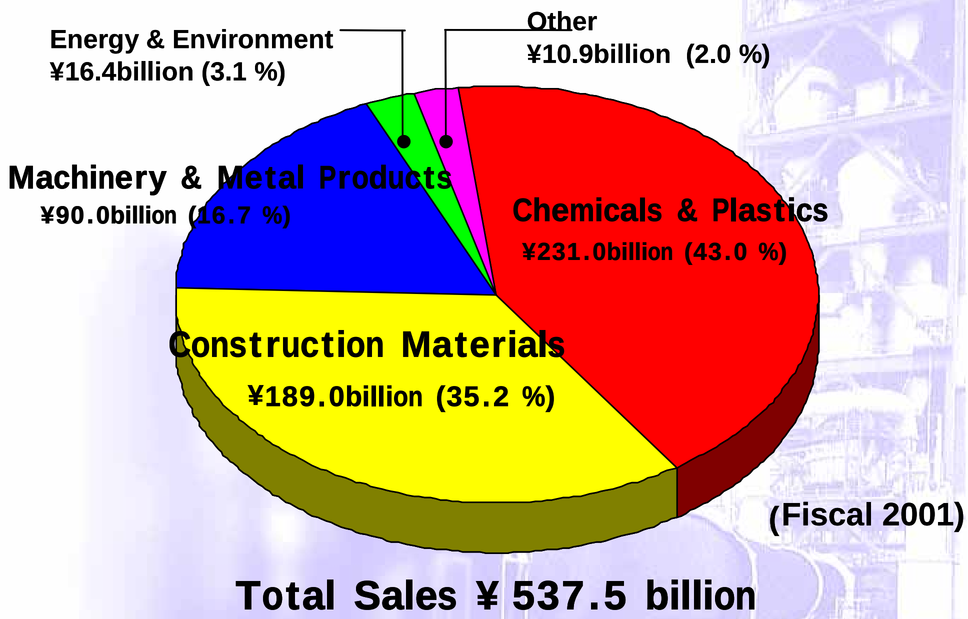
UBE INDUSTRIES,LTD.

Lines of Business

- Chemicals & Plastics
- Construction Materials
- Machinery & Metal Products
- Energy & Environment





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High Temperature Process in UBE

Coal Gasification Process

Waste Plastics Gasification Process

Aluminum Wheel for Automobile

Coal Center

Coal fired Power Plant

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Cement Factories in UBE

Kanda Cement Factory

Isa Limestone Mine
and Cement Factory

Ube Cement Factory

UBE Private Highway

Practical Applications of FactSage in UBE

ChemApp™ for ASPEN PLUS

Cement Production Process

Rotary Kiln Simulator
KilnSimu

Magnesia Clinker
Production Process

Power Plant
pulverized coal combustion
bio-mass combustion

Ash behavior in boiler
Bio-mass Ash behavior

FactSage™

Coal Gasification

Estimation of Slag
Melting Temperature

Waste Plastics Gasification

Chemicals Production
moving bed process

ChemApp™ for ASPEN PLUS
ChemSheet™

Environment Process
+ DIOXN
PCB database

Aluminum Wheel Production
for Automobile

ChemSheet™
+ Fslight database

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Cement Making Process

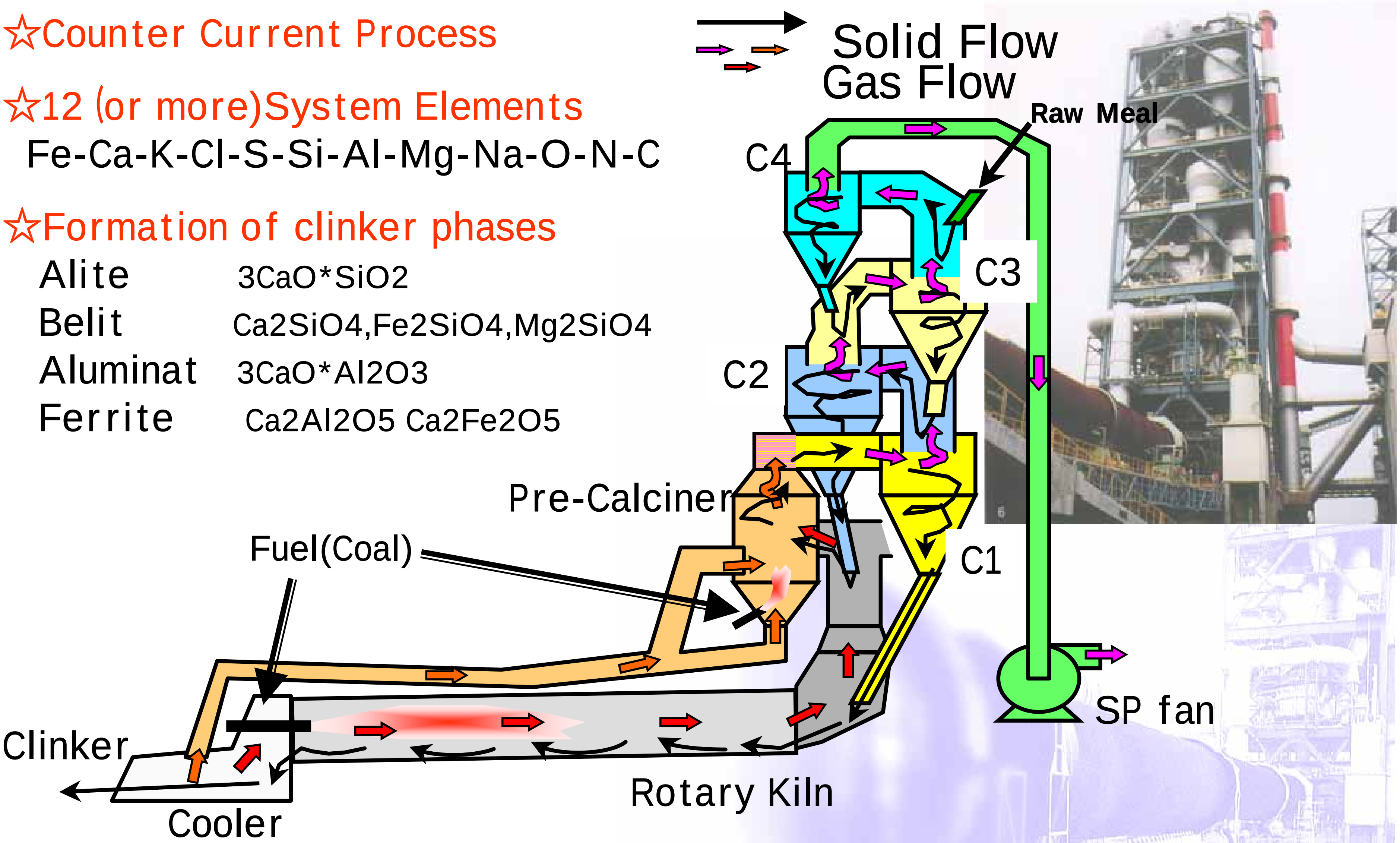
☆Counter Current Process

☆12 (or more)System Elements

Fe-Ca-K-Cl-S-Si-Al-Mg-Na-O-N-C

☆Formation of clinker phases

Alite	3CaO*SiO2
Belit	Ca2SiO4,Fe2SiO4,Mg2SiO4
Aluminat	3CaO*Al2O3
Ferrite	Ca2Al2O5 Ca2Fe2O5



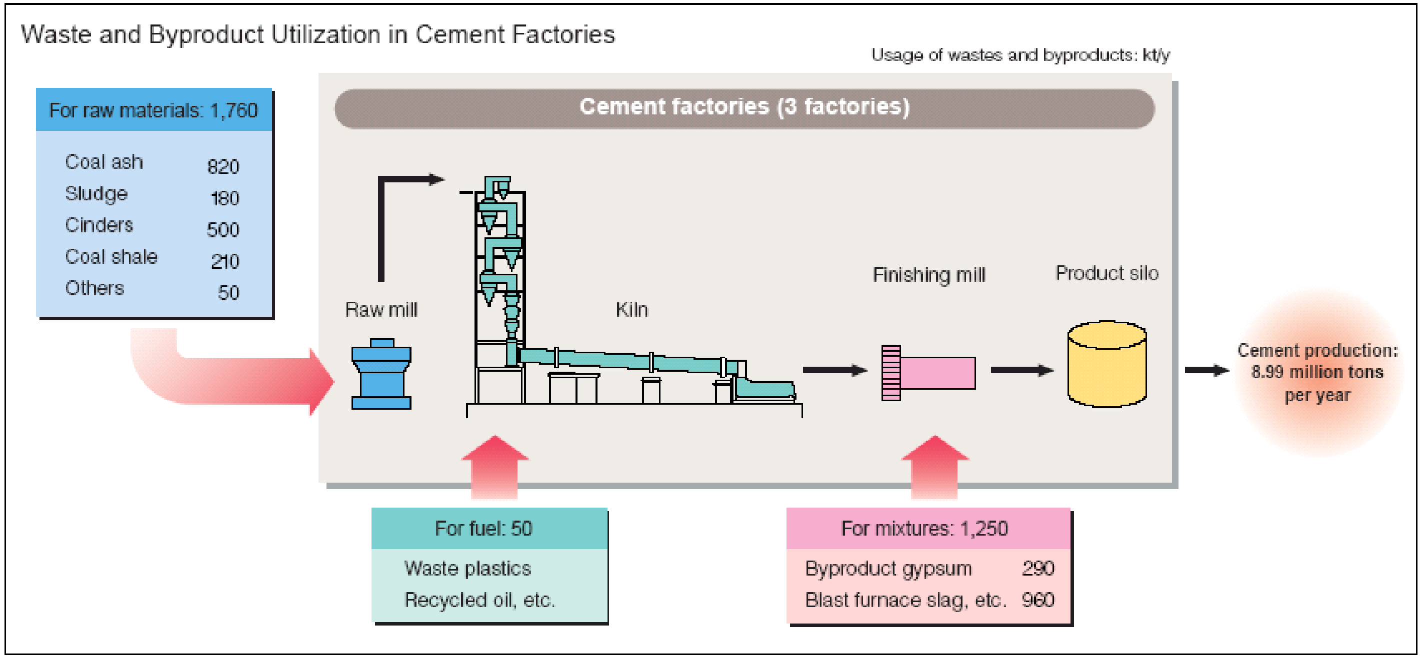
Waste and Byproduct Utilization in Cement Factories

Inorganic Waste(Raw)

Sewage
Public refuse incineration ash
Water supply sludge
Coal ash
Gypsum
Slag
Controlled soil
Hydraulic cake

Organic Waste(Alternative Fuel)

Waste plastics
Waste oil
Waste tire
Waste pachinko panels
Waste tatami mats
Bone meal

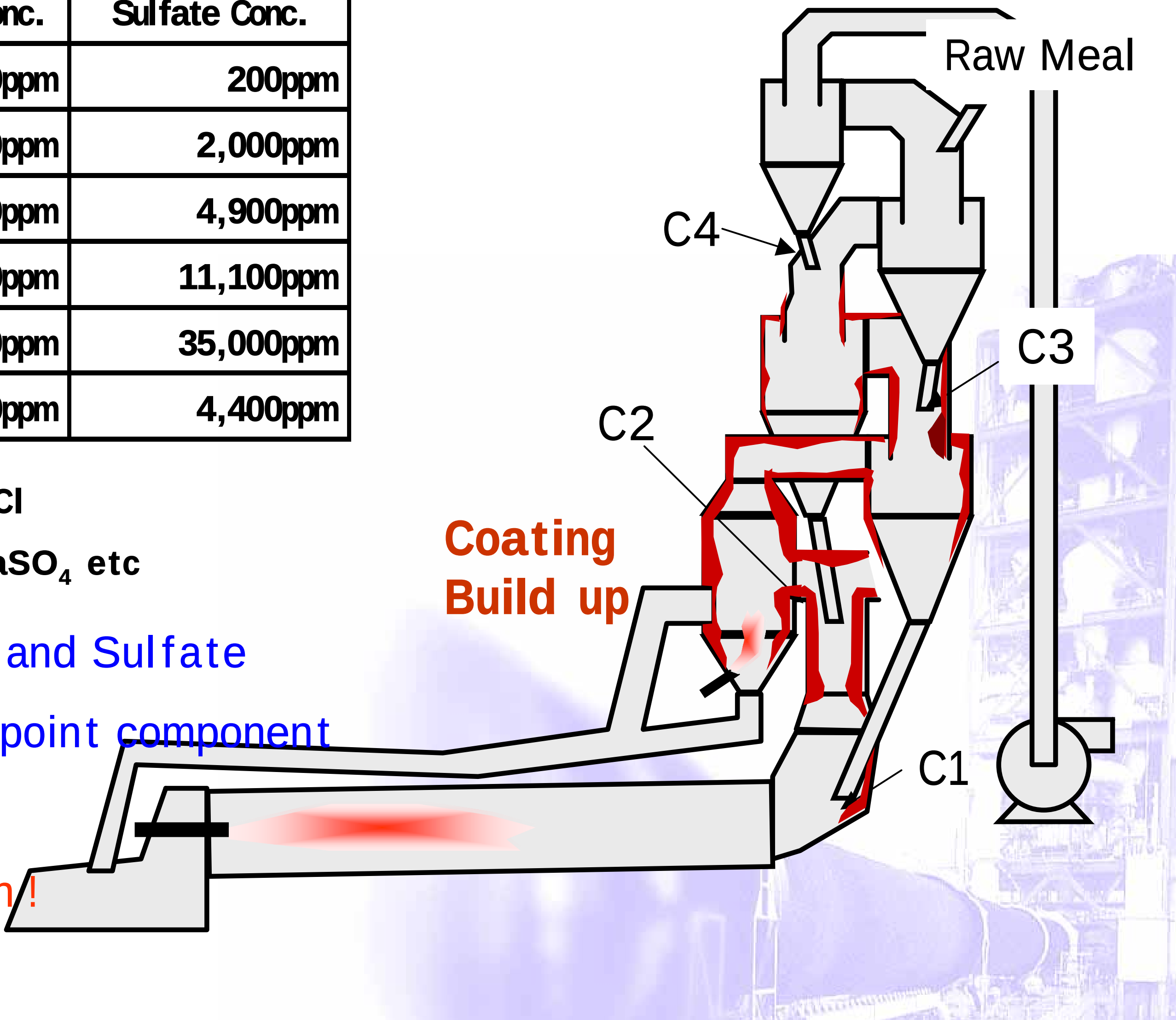


Cyclone clogging caused by Chloride and Sulfate accumulation

	Chloride Conc.	Sulfate Conc.
Raw Meal	60ppm	200ppm
C4	430ppm	2,000ppm
C3	840ppm	4,900ppm
C2	1,630ppm	11,100ppm
C1	11,880ppm	35,000ppm
Clinker	70ppm	4,400ppm

Chloride ;KCl, NaCl

Sulfate ;K_2SO_4,$CaSO_4$ etc



Accumulation of Chloride and Sulfate

⇩

Formation of low melting point component

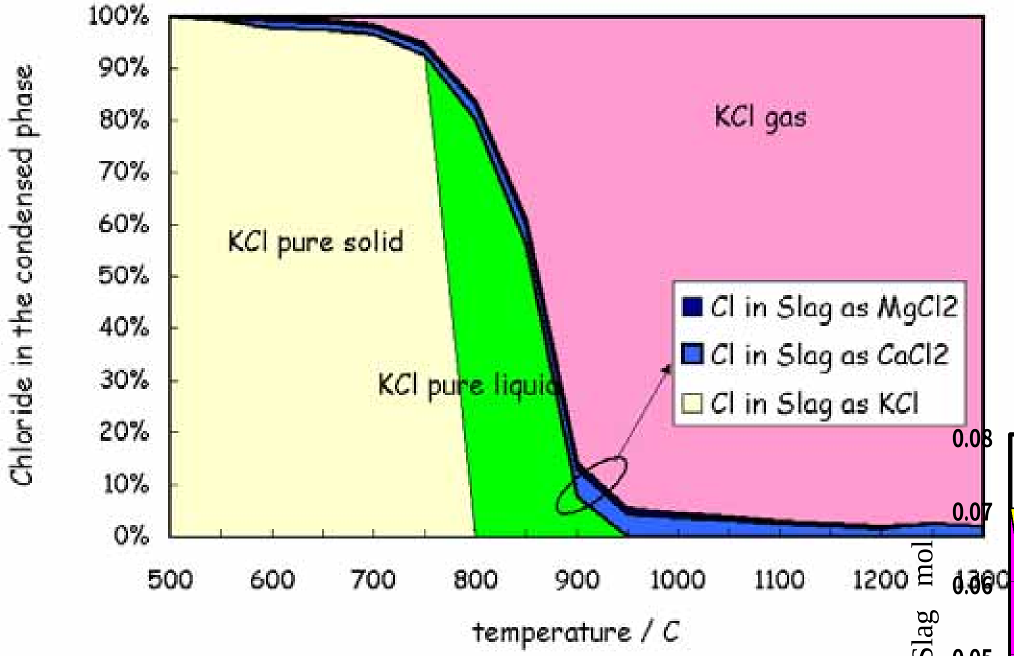
⇩

Cyclone clogging

⇩

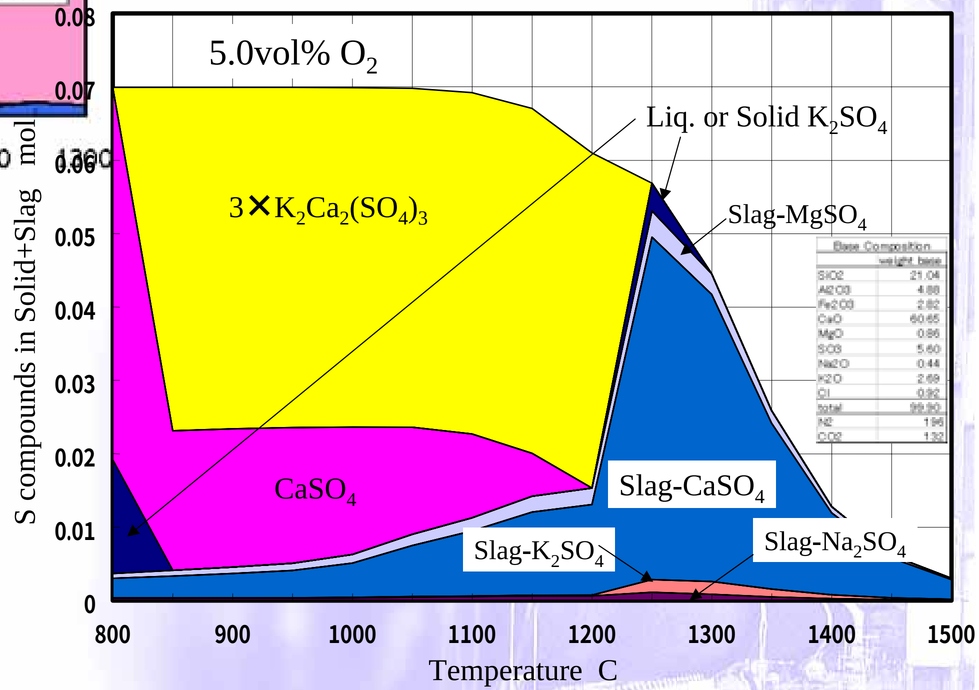
Plant Operation Shutdown!

Chloride and Sulfate at High Temperature

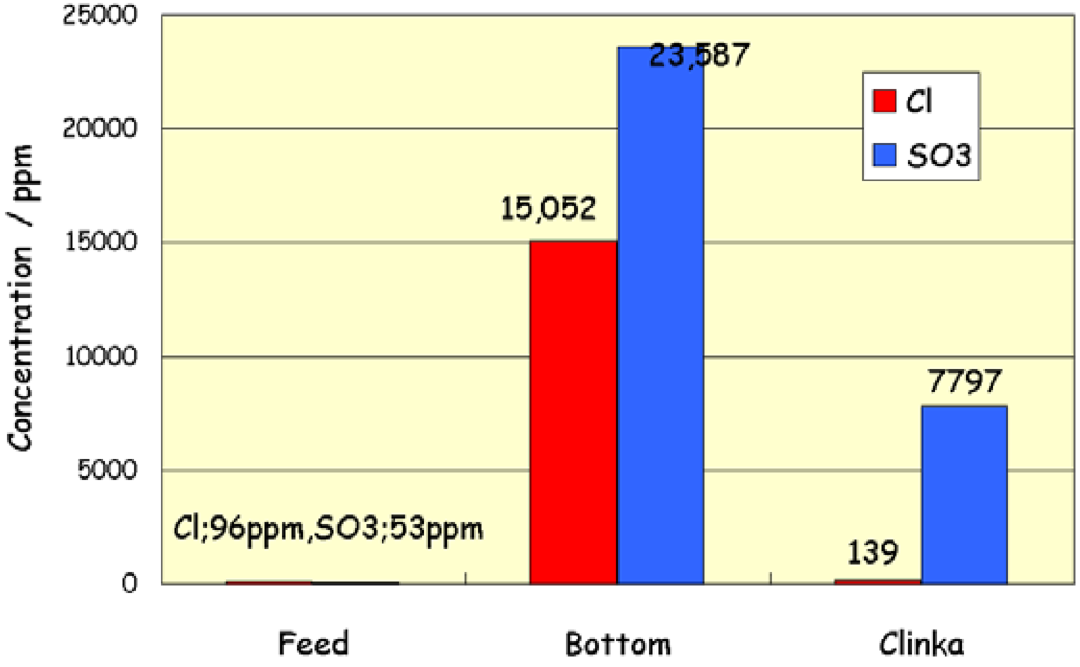


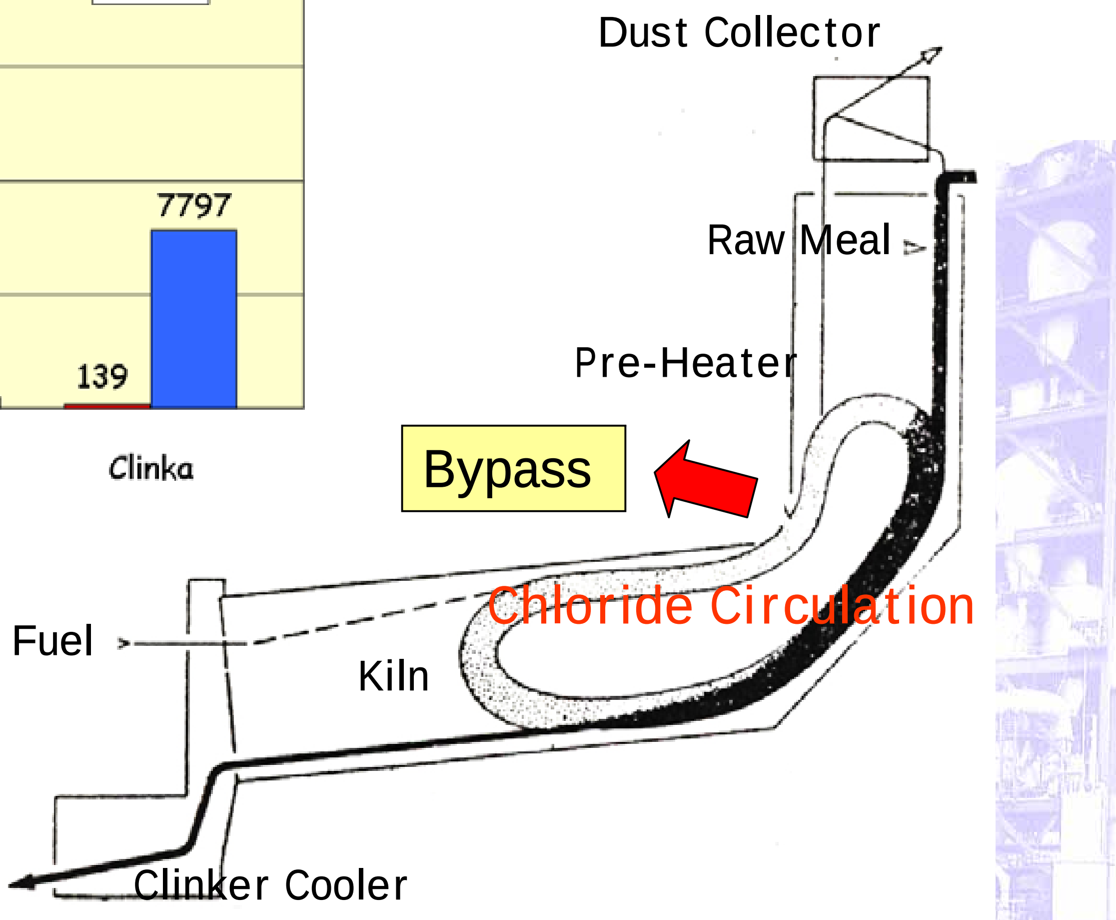
Chloride

Sulfate



Chlorine Bypass System





Process Simulation Tools

PC

OS	Windows XP
CPU	XEON 3.0GHz
RAM	2.75GB

Aspen Plus 2006

\+

V.5.3.2 for Aspen Pus

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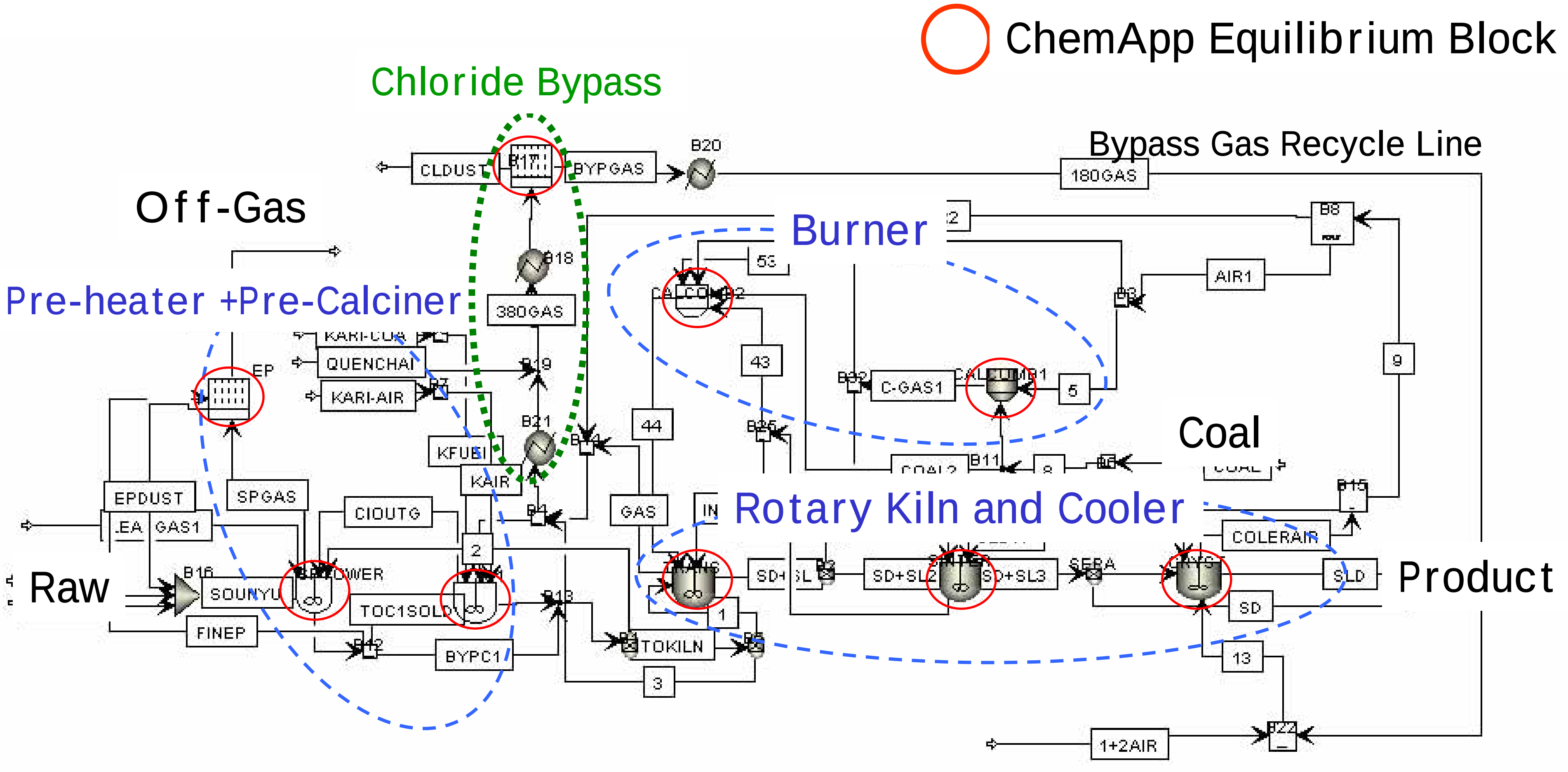
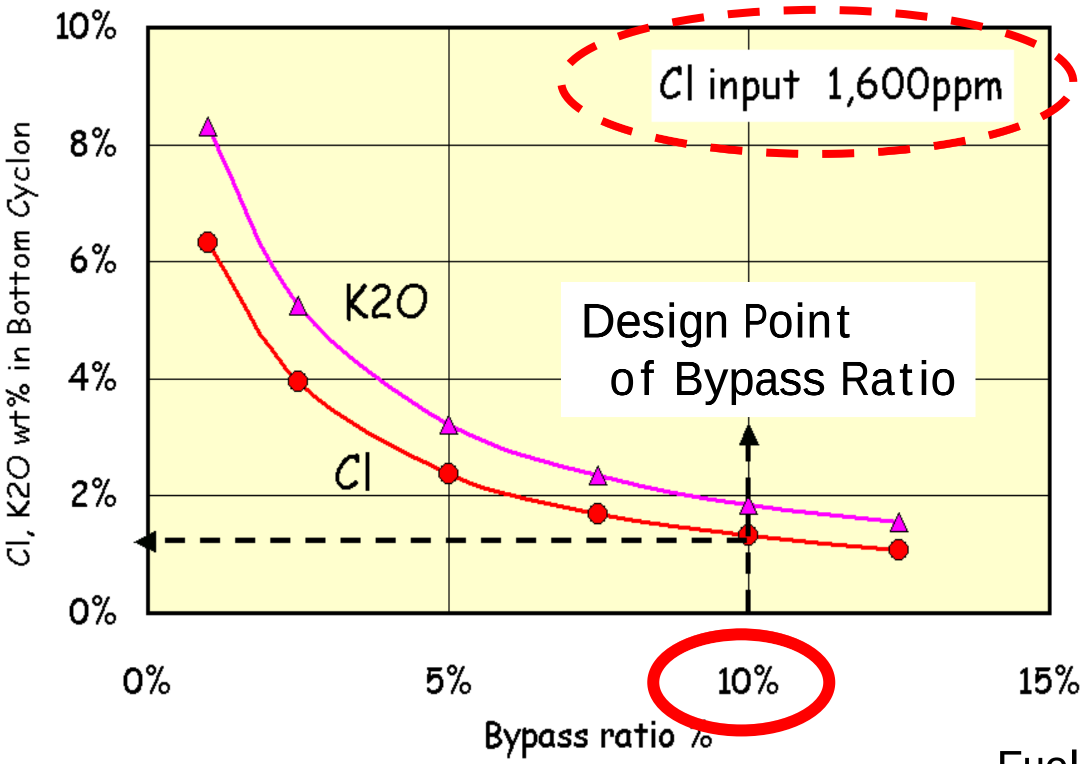
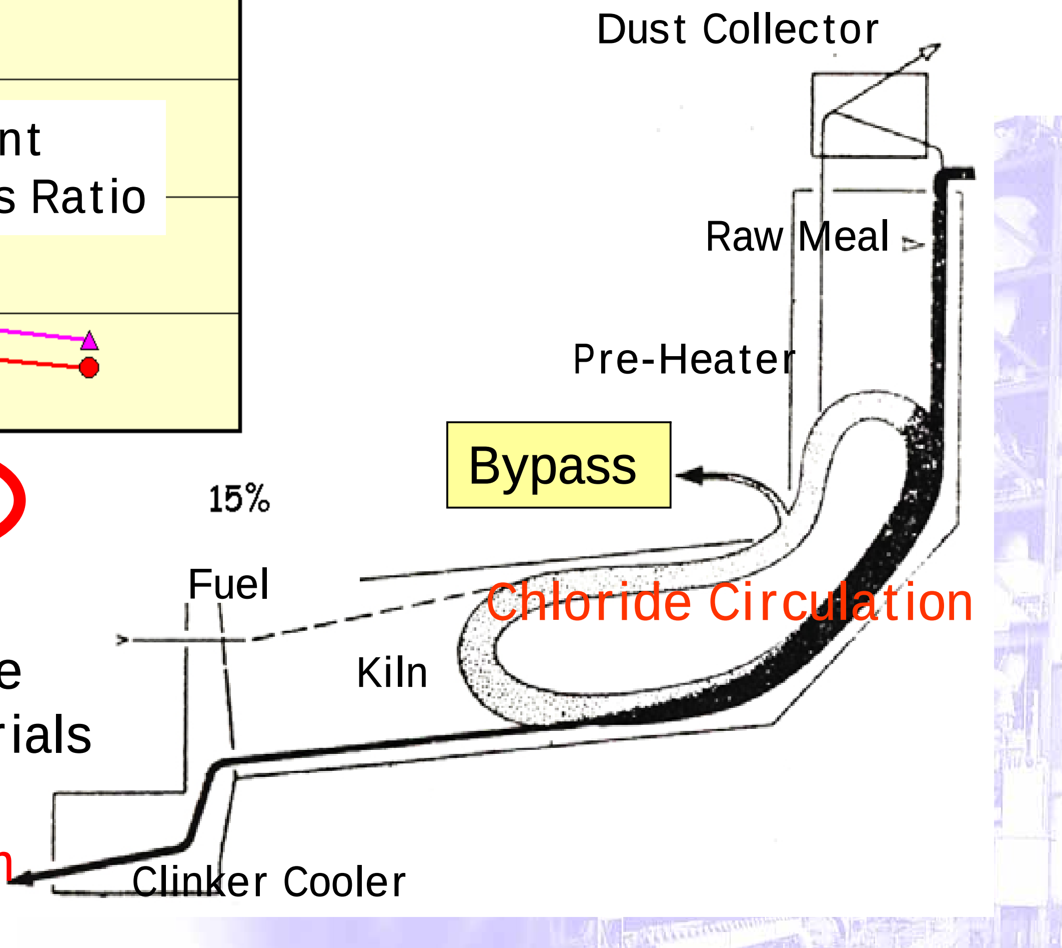
Aspen Plus model with Chloride Bypass System



High-Chlorine Bypass System





Chloride containing Waste can be used as an alternative raw materials

Allowable Limit of Cl is 1,600ppm per Clinker production

Solidification Analysis with ChemSeet

Squeeze Wheel®

- ✓ Solidification Analysis with correct thermodynamics
- ✓ Fitting Heat Transfer Coefficient

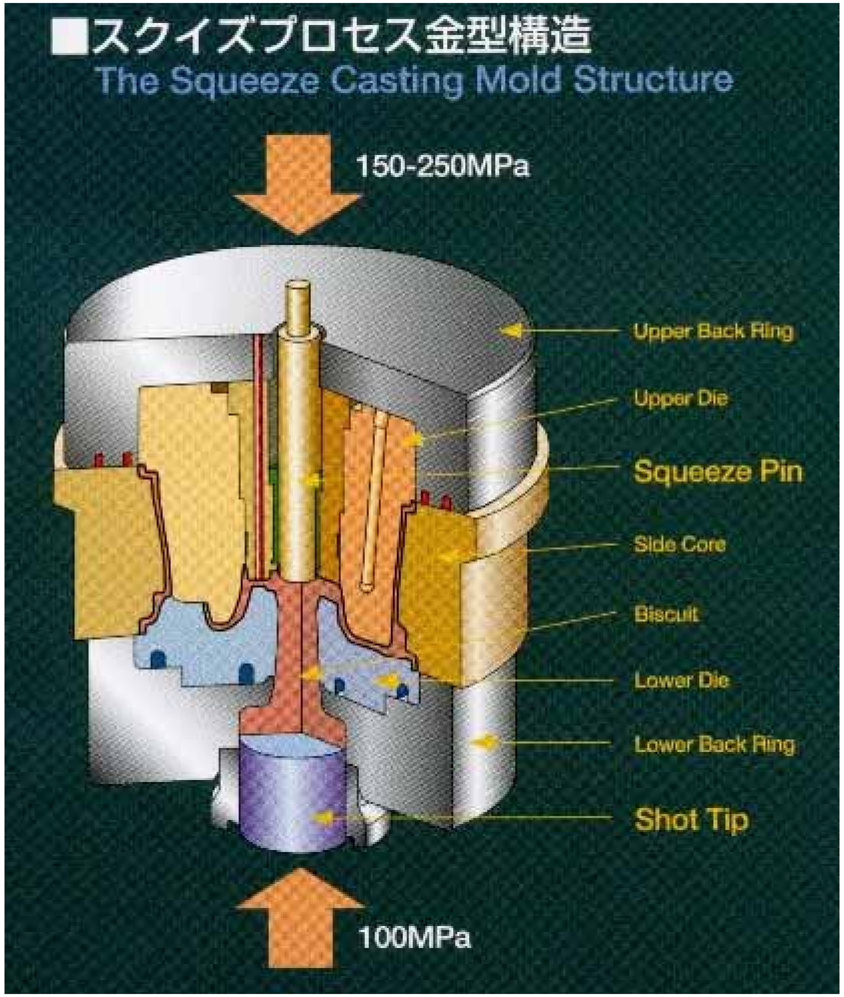
  Molten Metal / Die during solidification

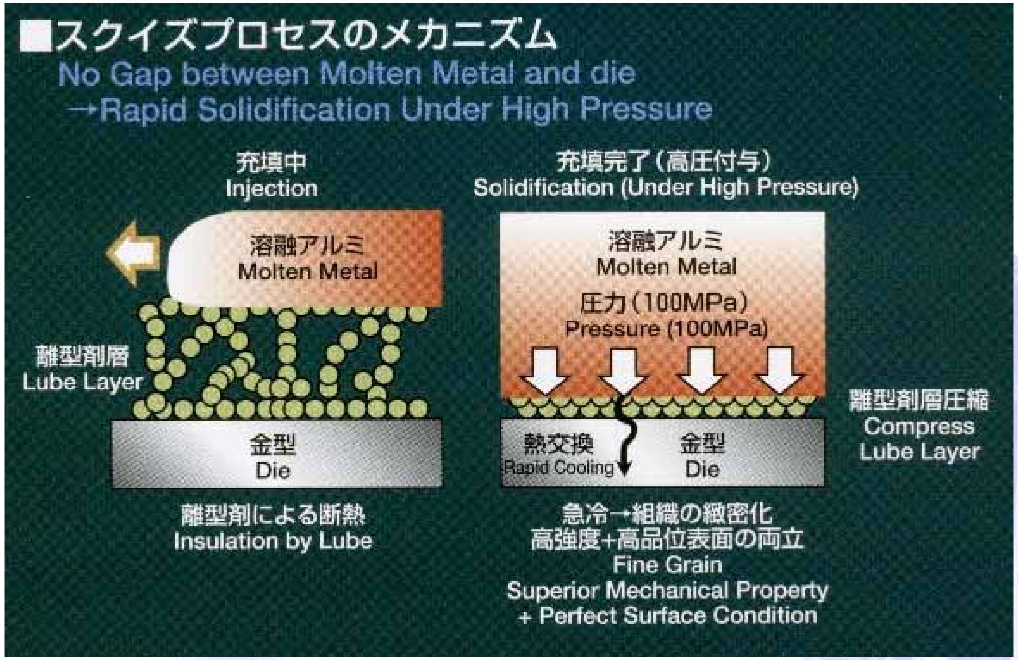
  Die / surroundings during die cooling
- ✓ Die temperature change with production cycle

Dynamic Simulation of Die Casting

"ChemSheet" + "FSlight light alloy database"

Squeeze Casting Process





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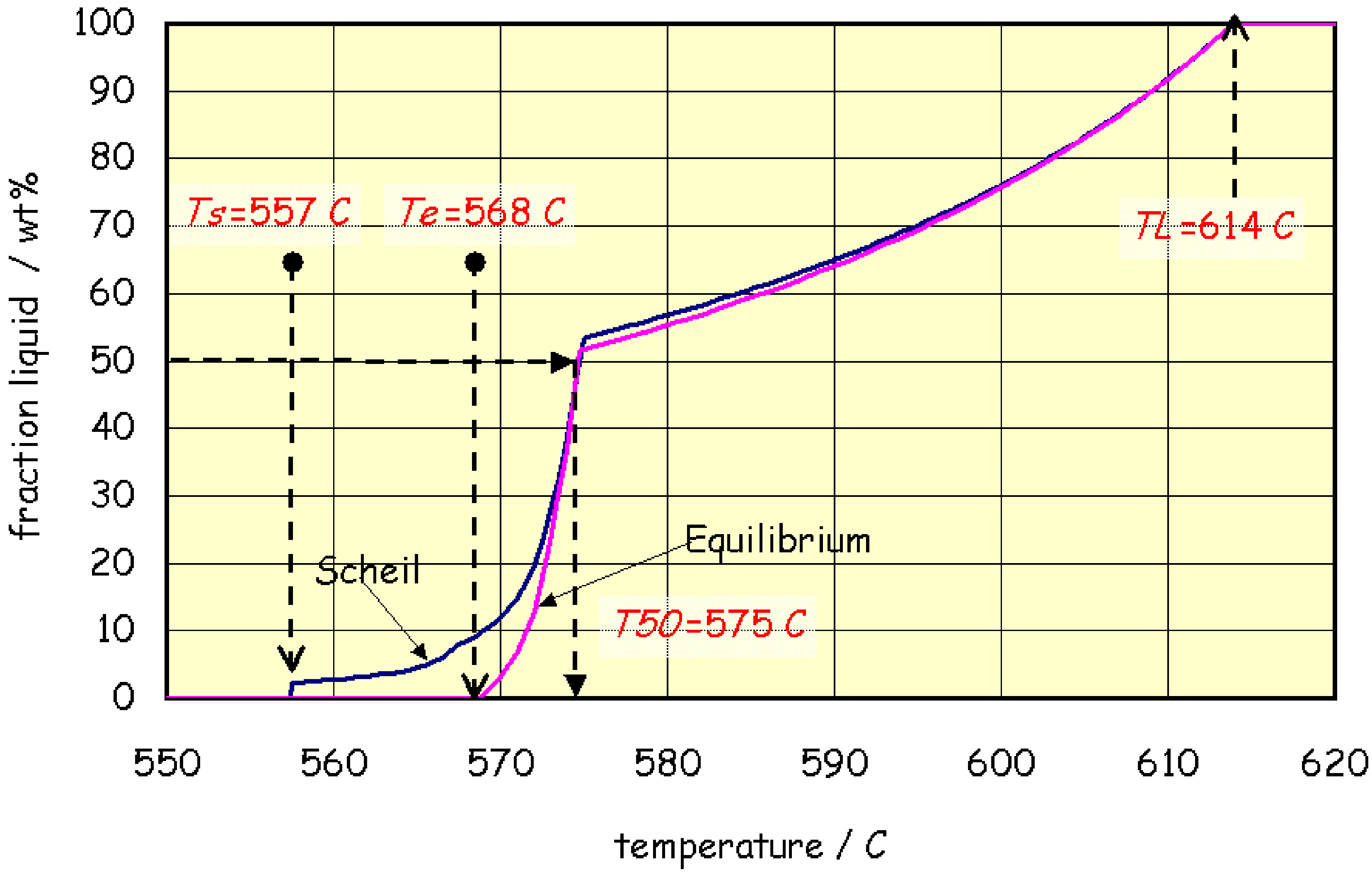
Solidification of Aluminum Alloy

AC4CH
Al ; 92.43, Si ; 7.20, Mg ; 0.24, Fe ; 0.13 wt%

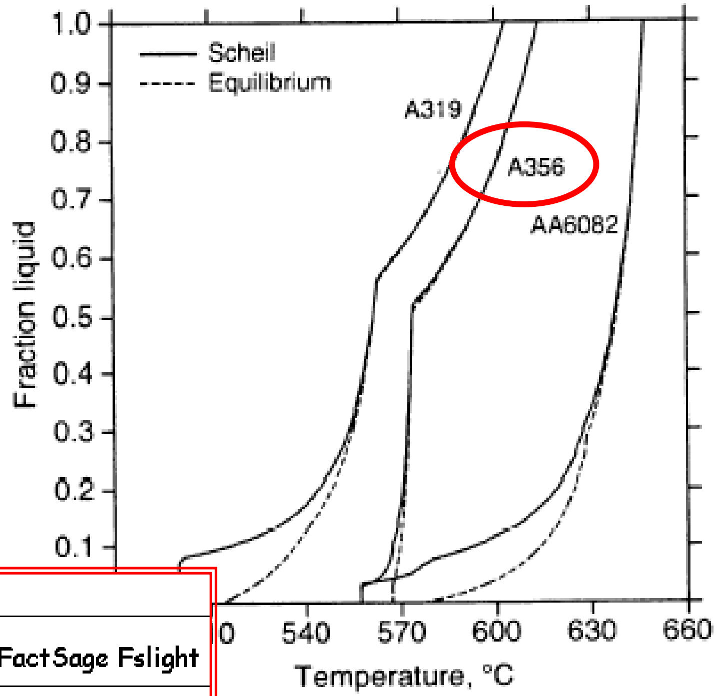


Comparison with Literature

Table 1. Chemical composition of the investigated aluminium alloys and steels according to charge analyses. Elements in parentheses were not considered in the simulations.

Alloy	Chemical composition, mass %										
	Al	C	Cr	Cu	Fe	Mg	Mn	Mo	Si	V	W
A356	Bal.	–	–	(0.01)	0.14	0.35	(0.01)	–	7.13	–	–
AA6082	Bal.	–	–	(0.07)	0.26	0.98	0.64	–	1.13	(0.01)	–
A319	Bal.	–	–	3.80	0.14	0.37	(0.02)	(0.02)			
100Cr6	–	1.0	1.49	–	Bal.	–	(0.34)	(0.011)			
HS6-5-2	–	0.86	4.05	–	Bal.	–	(0.29)	4.59			
X210CrW12	–	2.18	11.64	–	Bal.	–	(0.29)	(0.11)			

"Thermodynamic Criteria for the Selection of Alloys Suitable for Semi-Solid Processing"
,Evgueni Balitchev, et al, Material Chemistry, RWTH Aachen University



	Al	Si	Mg	Fe	TL	Te	Ts	T50	
AC4CH	92.43	7.20	0.24	0.13	614	568	557	575	FactSage Fslight
A356	92.38	7.13	0.35	0.14	614	567	557	574	Thermocalc

...id as function of temperature for the aluminium alloys A356, AA6082 and A319. Solid lines show Scheil–Gulliver calculations and dashed lines show equilibrium calculations. Small kinks are visible at fairly regular temperature intervals in the Scheil–Gulliver calculations. These are numerical artefacts and do not indicate a change of phases present.

Solidification and Die cooling model with ChemSheet

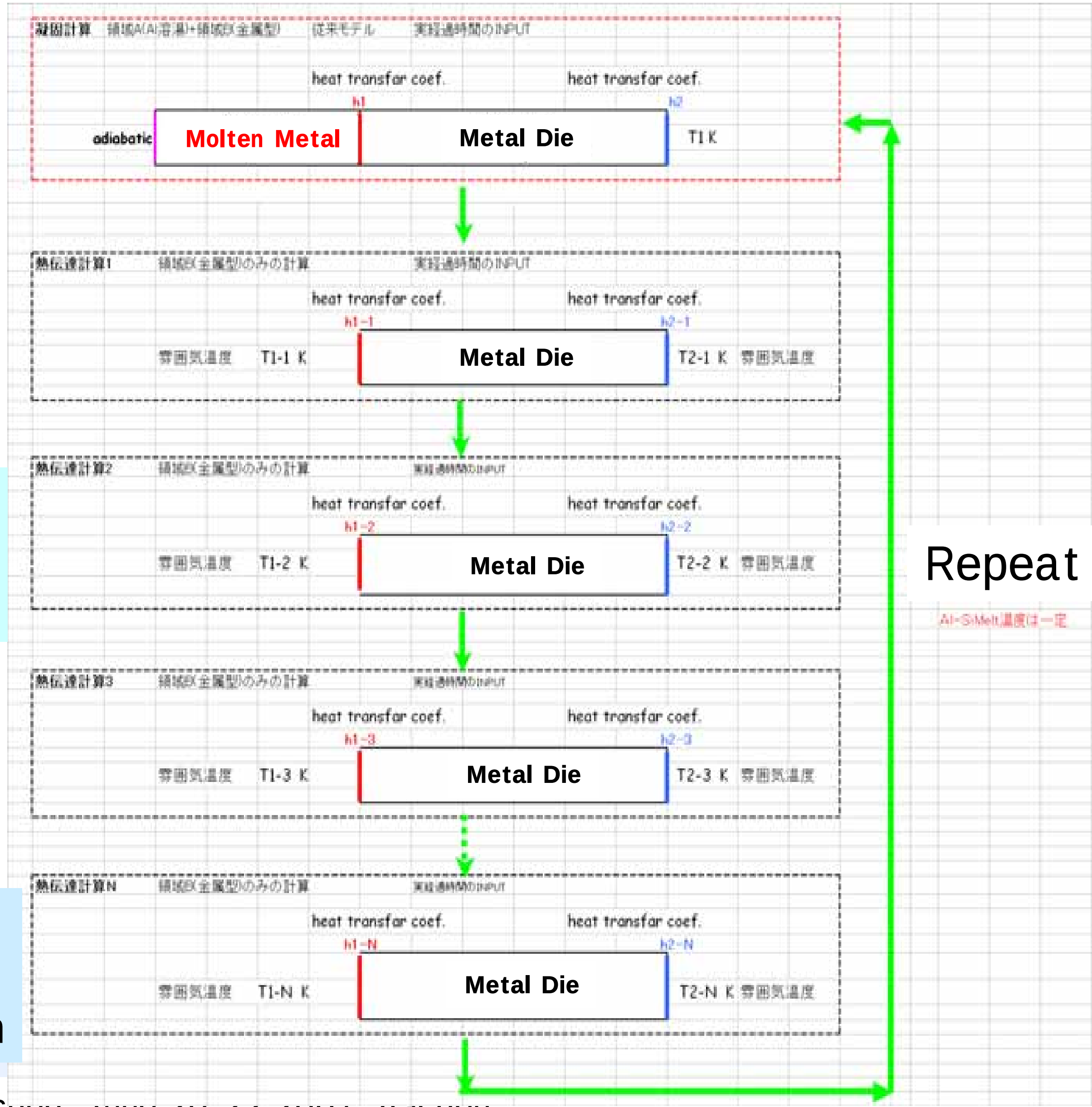
Molten Metal Injection and Solidification

Die Cooling-1
Pressure release

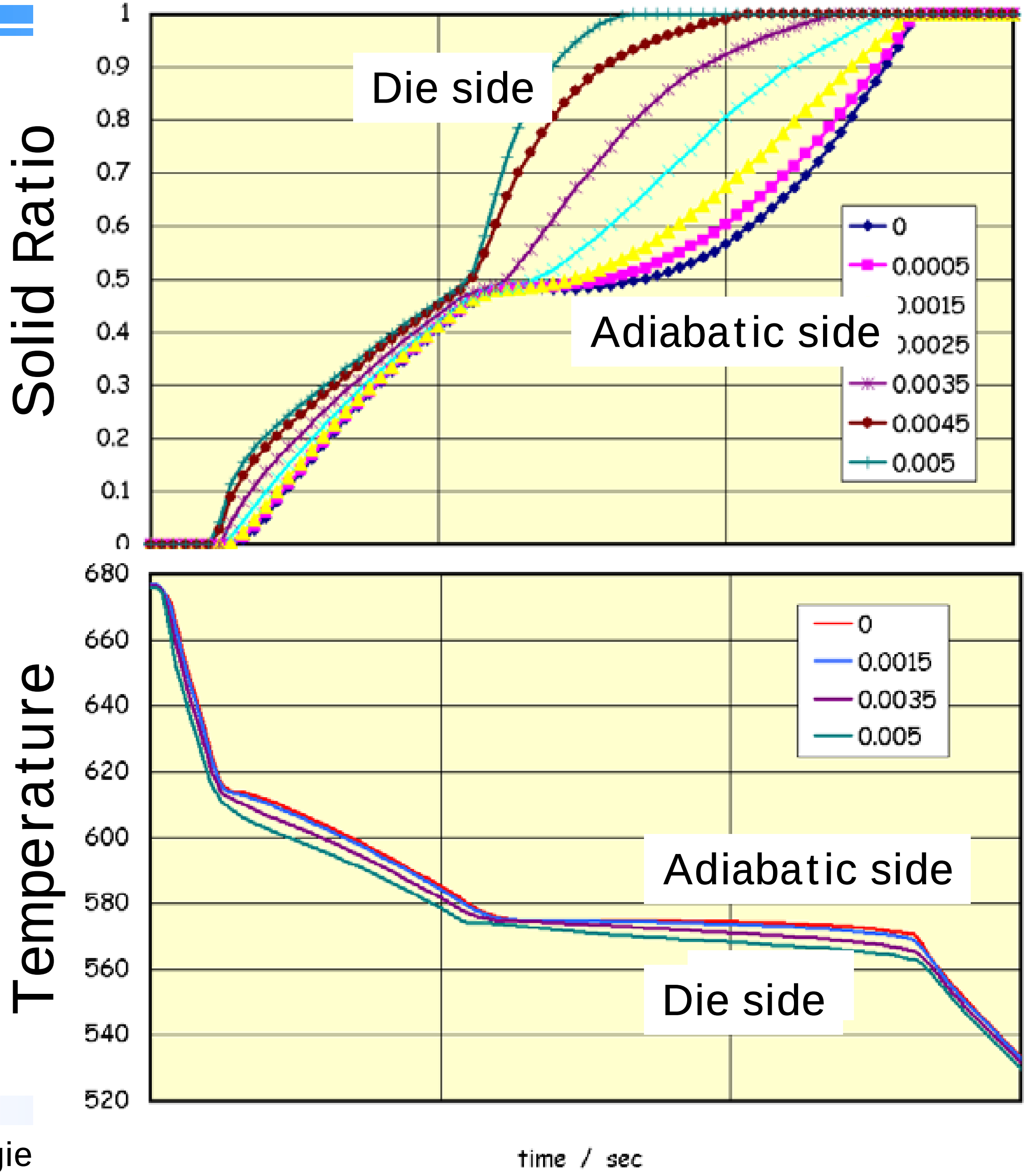
Die Cooling-2
Cooling
Natural Convection

Die Cooling-3
Cooling
Lubricant Splay

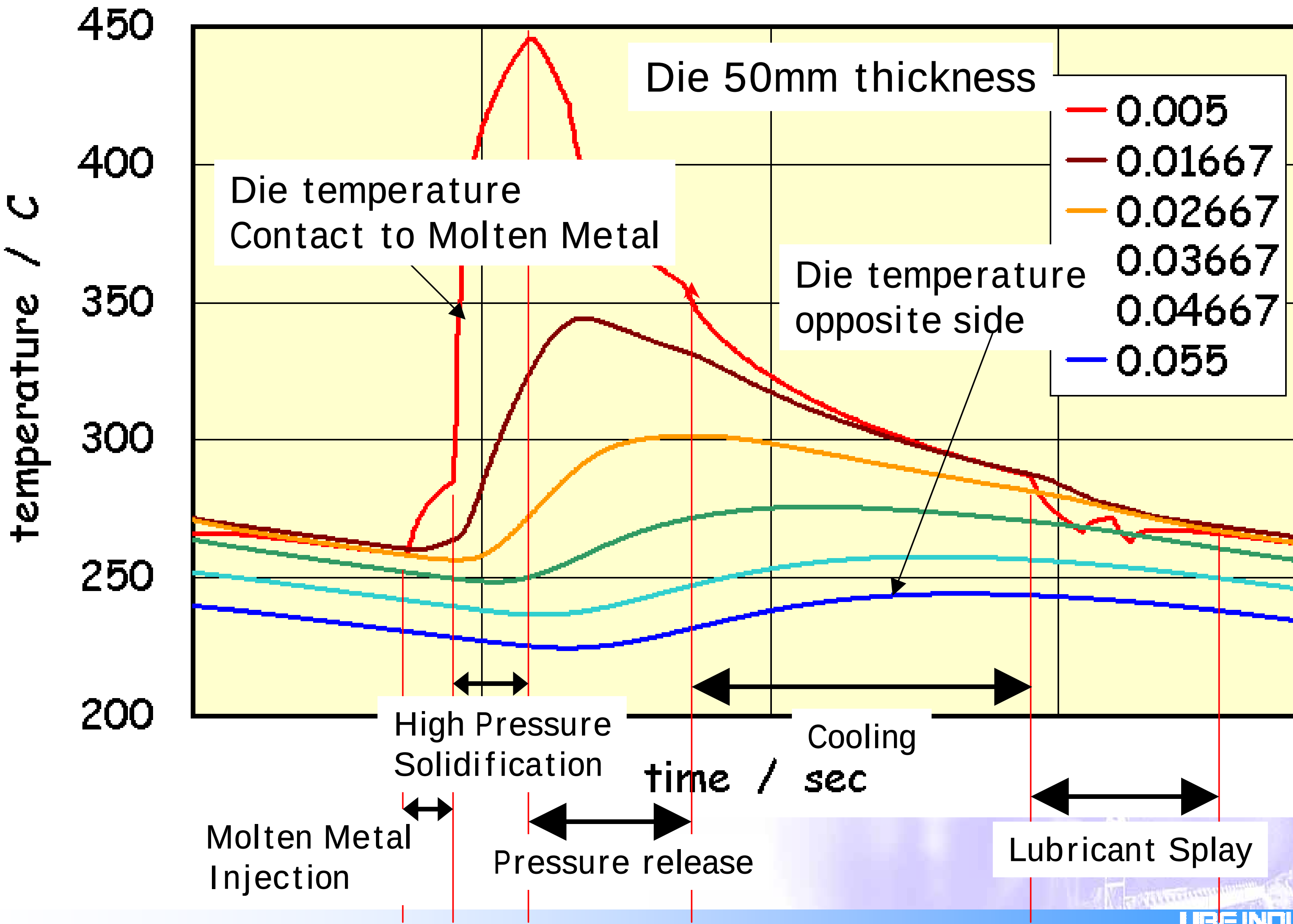
Die Cooling-4
Cooling
Natural Convection



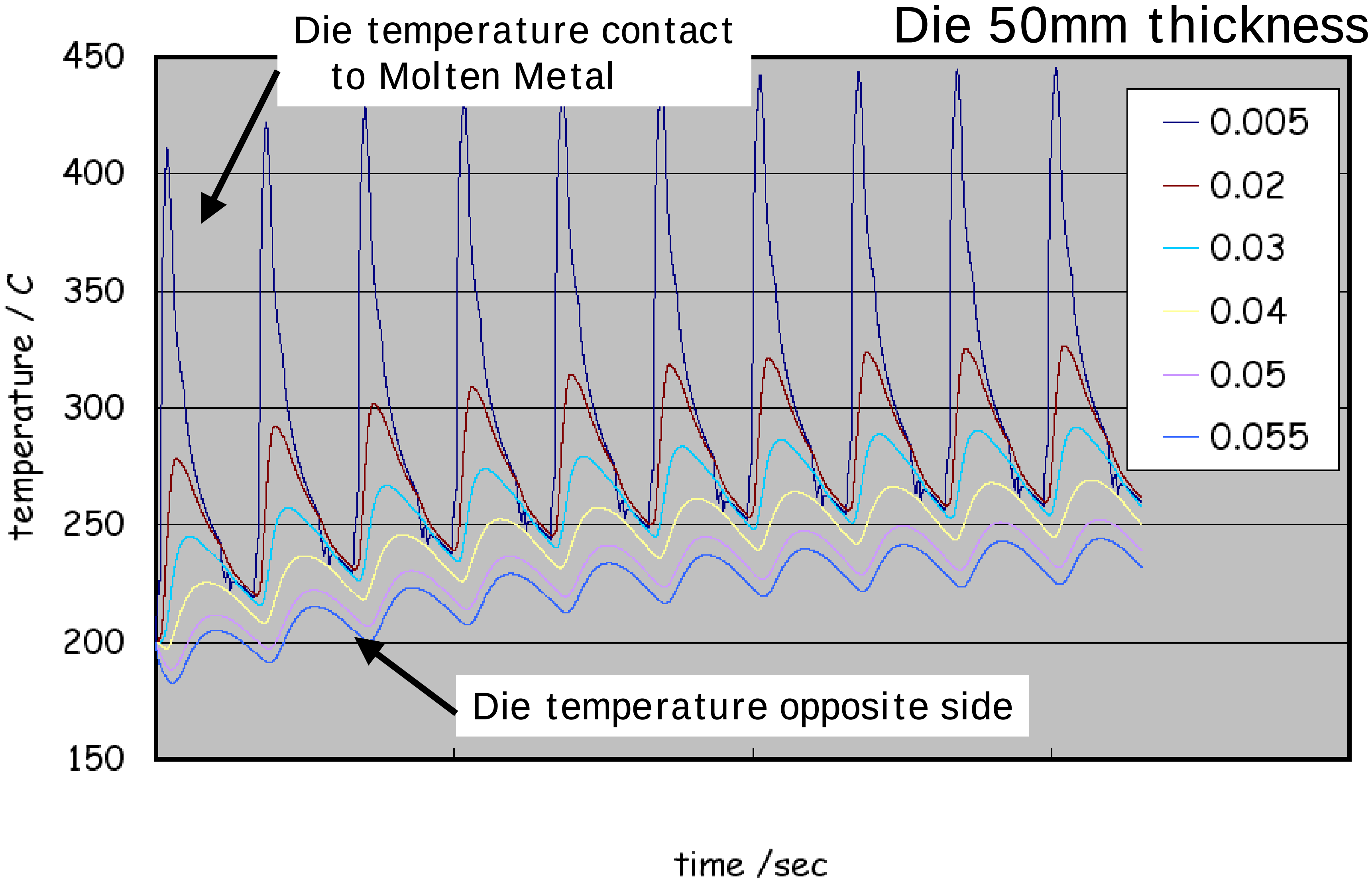
Solidification and Temperature change



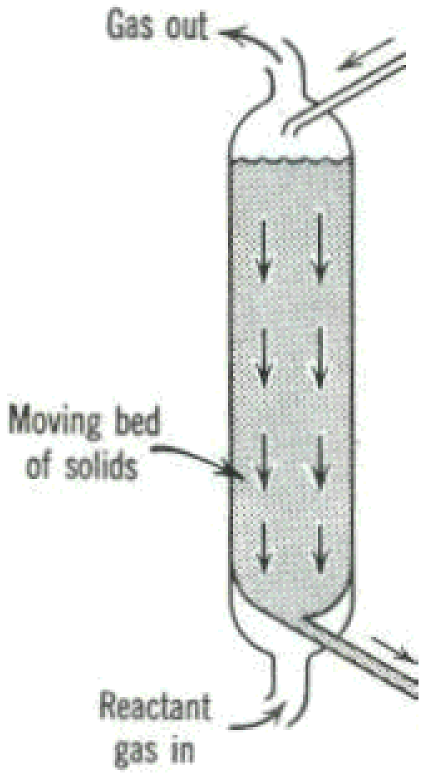
Temperature Profile of Die in One Cycle

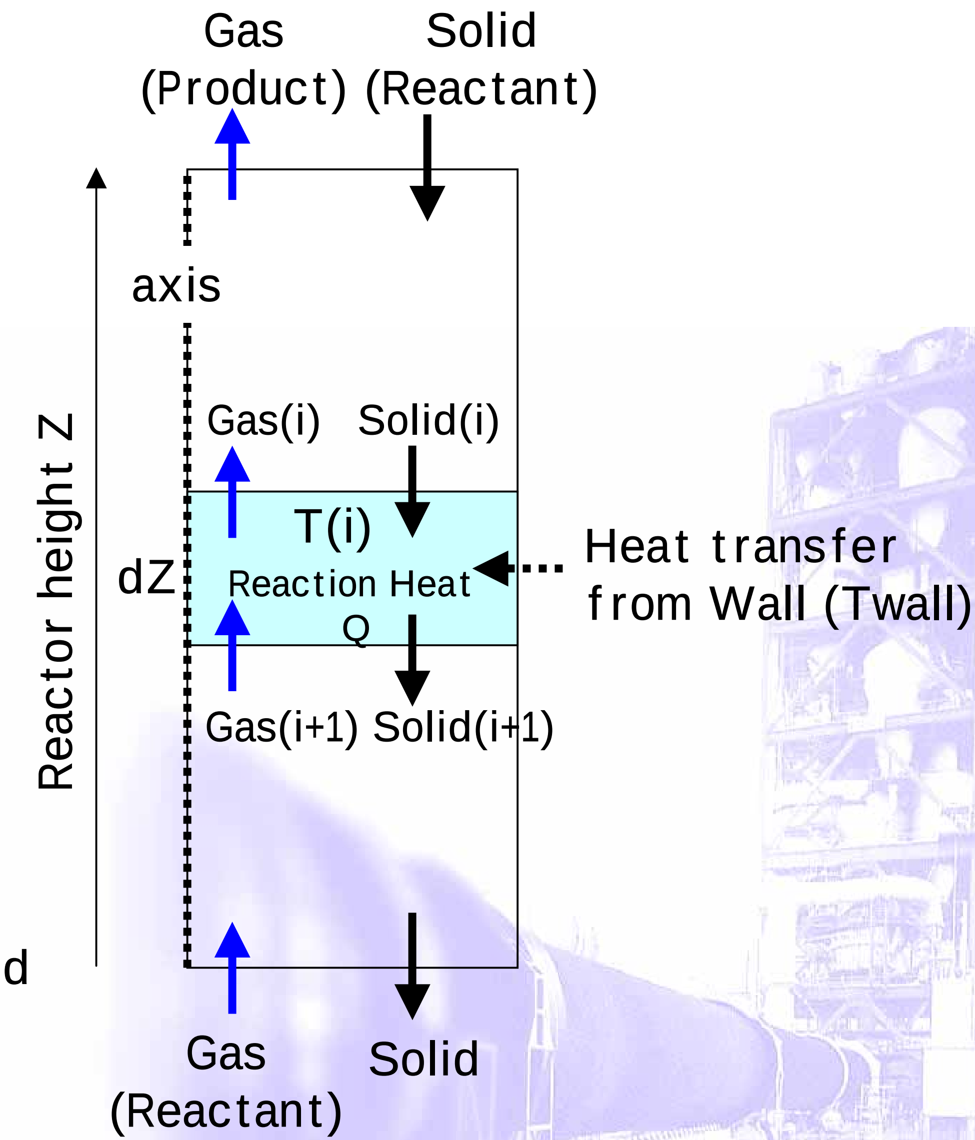


Die Temperature during Production Cycle



Modeling of “Moving Bed Reactor”





Assumption of Modeling
- No temperature difference Gas/Solid
- One dimensional(height) Model

Specification of ChemApp Block

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✓Subroutines | ✓User Arrays | **Configured Variables** | Calculation Options | Stream Flash

Configured variables

Label	Value
CALC_TYPE_1_TO_4	1
SPEC_PRESSURE_PA	101325
SPEC_T_Q_OR_TMIN	1100
SPEC_TMAX_OPTION	
NO_OF_TARG_1_MAX	0
NO_OF_PHASE_IDS	1
PHASE_IDS(1)	SLAG
NO_OF_COMP_IDS	273
COMP_IDS(1)	H:G1
COMP_IDS(2)	H2:G1
COMP_IDS(3)	N:G1
COMP_IDS(4)	N2:G1
COMP_IDS(5)	N3:G1
COMP_IDS(6)	NH:G1
COMP_IDS(7)	NH2:G-01

1; P,T
2; P,dH(W), incase of dH=0 adiabatic
3,4; Target calc.

Pressure;Pa

Temperature(K) in type1, dH(W) in type2

Number of Phase
in this sample only "Slag-liquid" was considered

Name of Phase

Number of Components

✓Define | ✓**Calculate** | ✓Sequence | Tears | Stream Flash | EO Options

Calculation method
- (●) Fortran
- ( ) Excel

Fortran Declarations

Enter executable Fortran statements

```
F      PPFACT_FILEN = 'pbzn.CST'
F      PPFACT_CADBG =  .false.
```

definition of cst file name

ChemApp Reactor Block with Heat Transfer

UBE

ChemApp Block has only 2 mode !

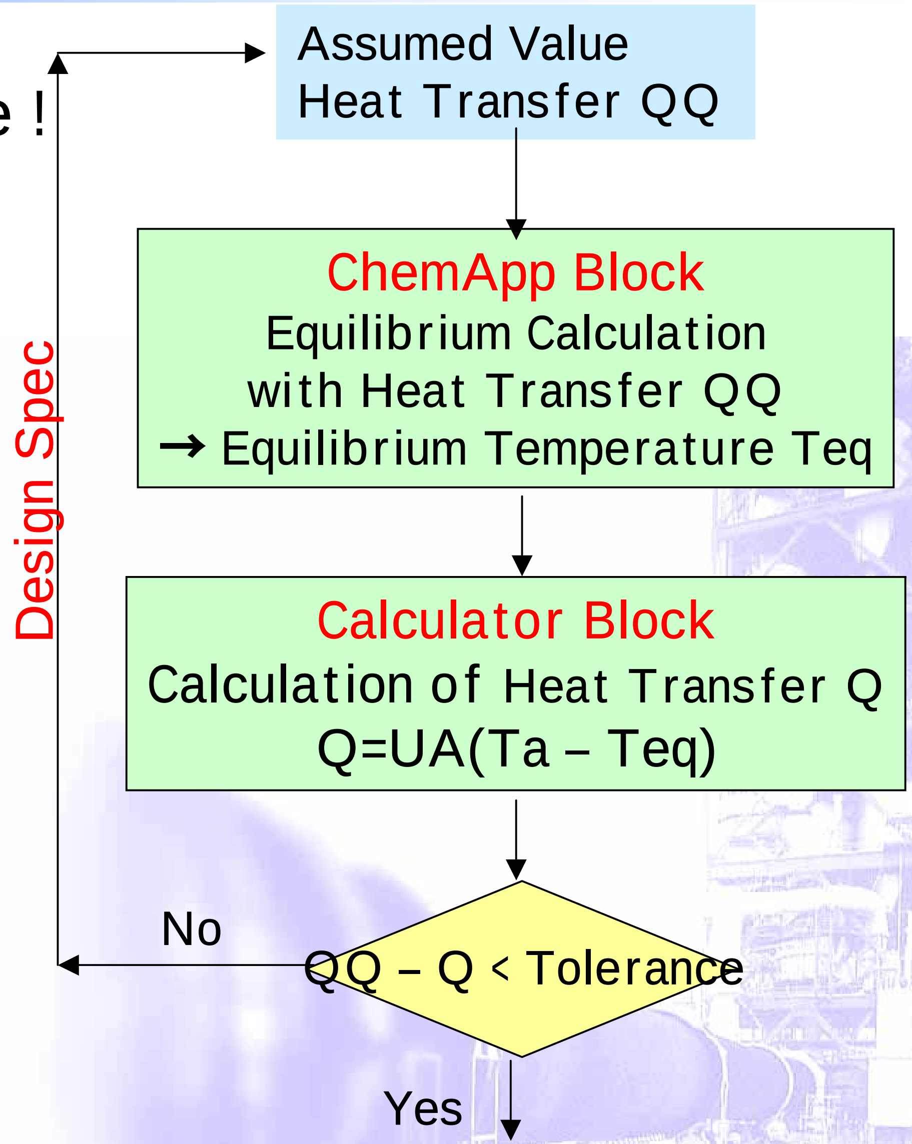
- Constant Temperature
- Constant Heat Flow

ChemApp Calculation with heat transfer

Q = UA(Ta – Teq)

U ; Heat Transfer Coefficient
A ; Heat Transfer Area
Ta ; Surrounding Temperature

Teq ; Reactor temperature



Input of "Calculator" and "Design Spec"

UBE

ASPEN PLUS "Calculator"

Valuable Definition

Define | Calculate | Sequence | Tears | Stream Flash | EO Options

Variable name	Info. flow	Definition
H1		Parameter Parameter no.=1 Physical type=Heat-Trans-C Units=kcal/hr-sqm-K
A1		Parameter Parameter no.=2 Physical type=Area Units=sqm
Q1		Parameter Parameter no.=3 Physical type=Enthalpy-Flo Units=kcal/hr
DIA		Parameter Parameter no.=100 Physical type=Length Units=meter
L		Parameter Parameter no.=101 Physical type=Length Units=meter
T1		Stream-Var Stream=S-1-OUT Substream=CISOLID Variable=TEMP Units=K
TS1		Parameter Parameter no.=4 Physical type=Temperature Units=C
TT1		Parameter Parameter no.=5 Physical type=Temperature Units=C

Calculation of Heat Transfer Q

Define | Calculate | Sequence | Tears | Stream Flash | EO Options

Calculation method: (•) Fortran ( ) Excel

Fortran Declarations

Enter executable Fortran statements

```
C  H1 = heat transfer coef ; kcal/m2/hr/K
C  A1 = area              ; m2
C  Q1 = heat flow         ; kcal/kr
      H1 = 30
      TS1 = 300
      DIA = 0.55
      L = 1.5
      A1 = DIA**2*3.1415/4*L
      TT1 = T1-273.15
      Q1 = H1*A1*(TS1-TT1)
```

ASPEN PLUS "Design Spec"

Valuable Definition

Define | Spec | Vary | Fortran | Declarations | EO Options

Flowsheet variable	Definition
QQ1	Block-Var Block=B1 Variable=REAL-VAR Sentence=REAL Element=2
Q1	Parameter Parameter no.=3 Physical type=Enthalpy-Flo Units=Watt

Convergence condition

QQ – Q < 0.1

Define | Spec | Vary | Fortran | Declarations | EO Options

Design specification expressions

Spec:	QQ1-Q1
Target:	0
Tolerance:	0.1

Vary QQ

Define | Spec | Vary | Fortran | Declarations | EO Options

Manipulated variable

Type:	Block-Var
Block:	B1
Variable:	REAL-VAR
Sentence:	REAL
Element:	2

Manipulated variable limits

Lower:	-1000
Upper:	1000
Step size:	
Maximum step size:	

Report labels

Line 1: Line 2: Line 3: Line 4:

EO input

Open variable:

Description:

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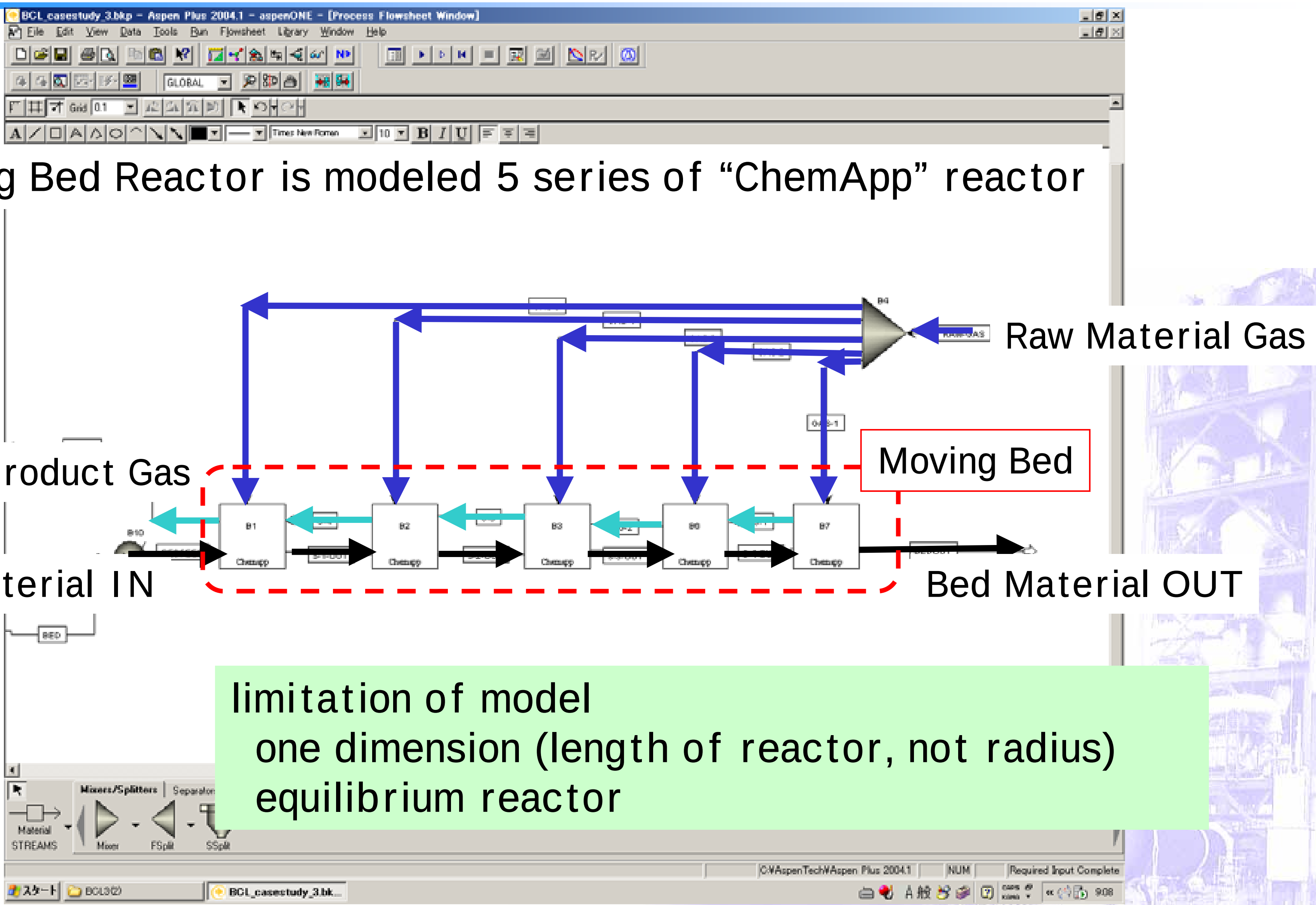
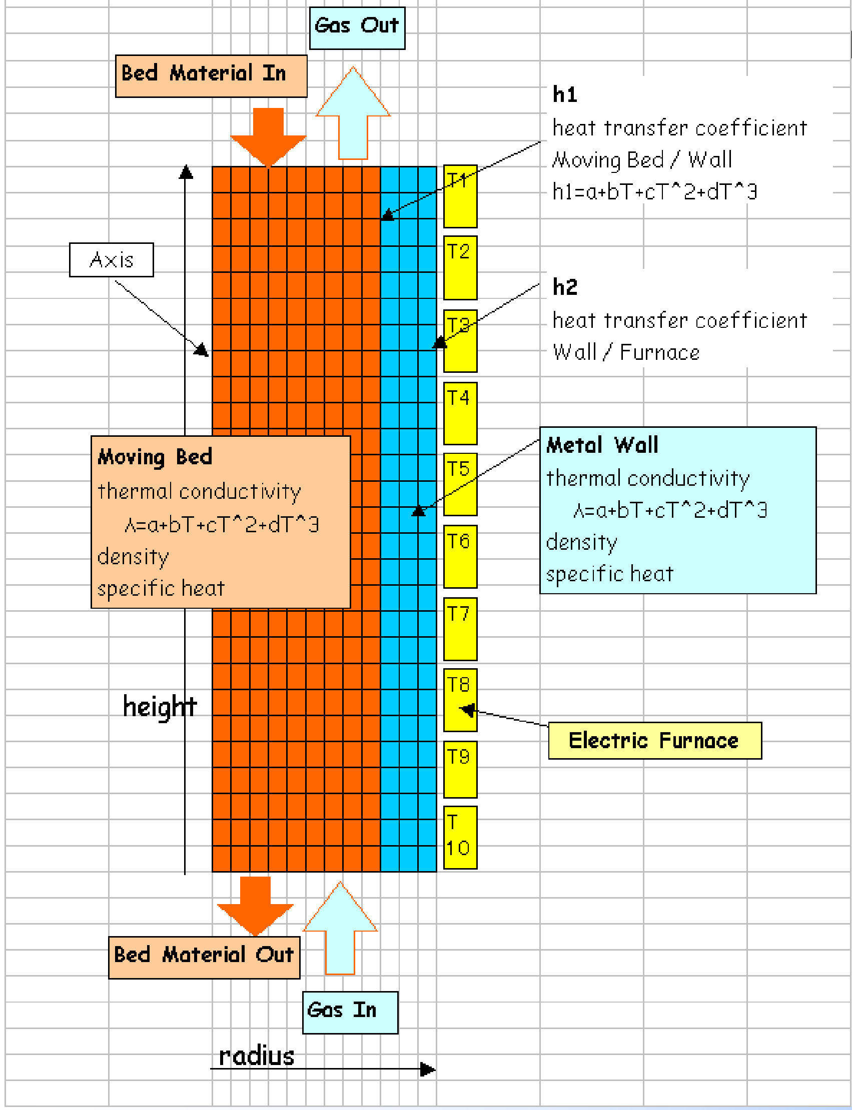
Modeling with Aspen Plus



limitation of model
- one dimension (length of reactor, not radius)
- equilibrium reactor

Moving Bed Model by “ChemSheet”

ChemSheet Model



ChemSheet Model is under development cooperation
with Mr. Fukayama, RCCM, Japan

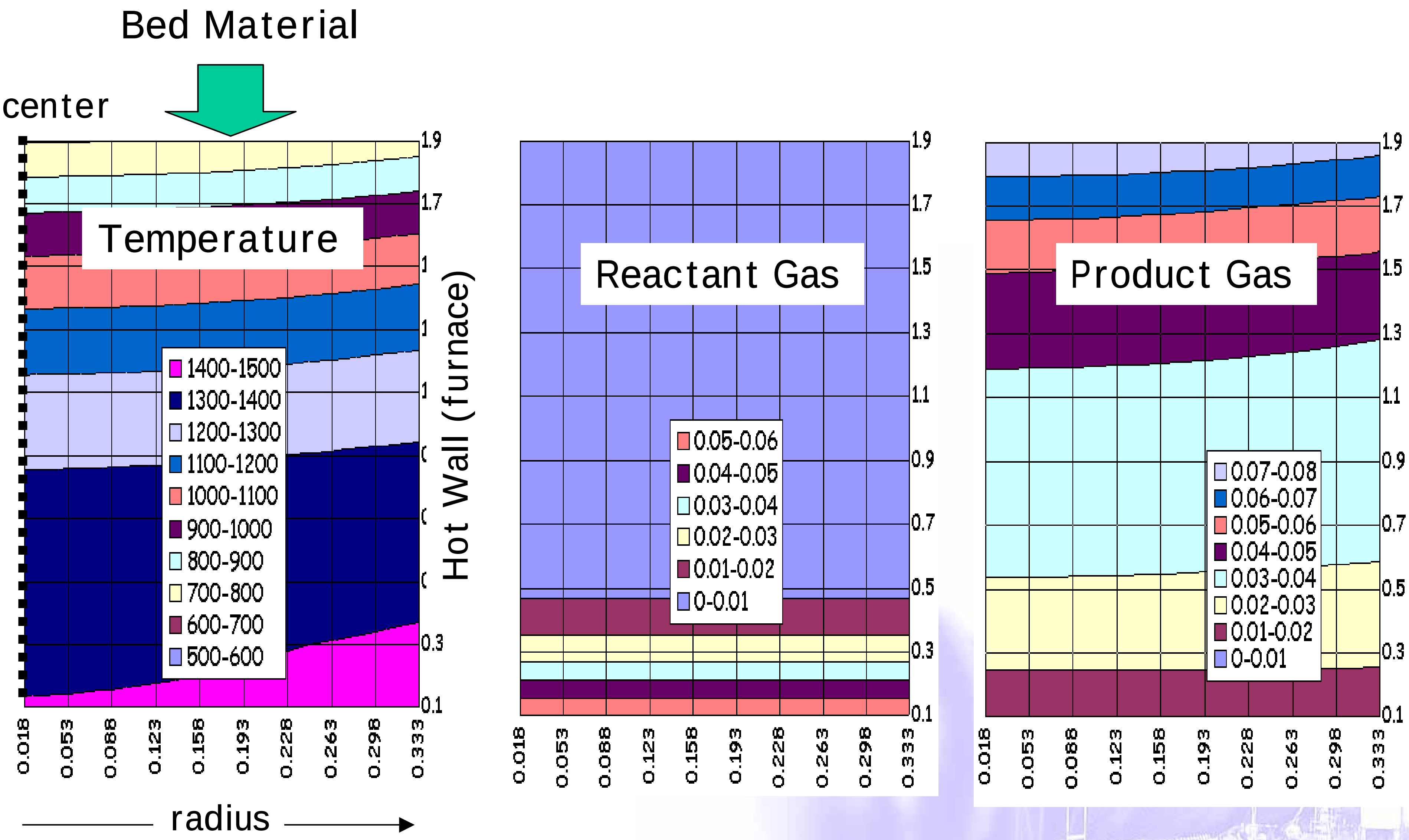
Model Topics

✓Some cells are set in Radius Direction
✓Restricted Equilibrium calculation at each cell

Advantage of ChemSheet Model

✓Radius Temperature Distribution in moving bed
✓Restricted Equilibrium calculation
✓Accurate estimation of Reactor Performance

Calculated Example



Wings of technology
Spirit of innovation

UBE