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Modeling of Clogging / Erosion of Nozzle Refractories

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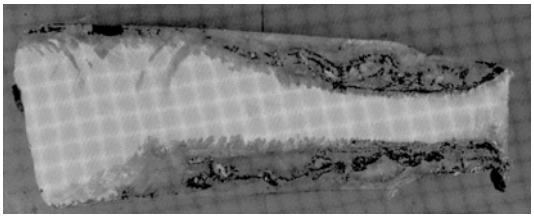
Presentation

- Problem statement
- Model Description
- Model equation derivations and validations
- Post processing
- Picking diffusion coefficients
- Results and estimations
- Summary

Problem Statement

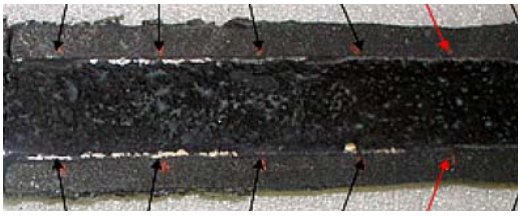
- Nozzle Clogging commonly plagues the steel industry
- Clogging and erosion leads to detrimental inclusions in the final product
- Many complex coupled phenomena govern the process: turbulent flow, multi-component multi-phase thermodynamics, ion-diffusion (in bulk, solid-phase, liquid-phase, and grain-boundaries), chemical reactions (eg. graphite oxidation, spinel formation, etc.)

Clogging (conventional Alumina-Graphite nozzle)



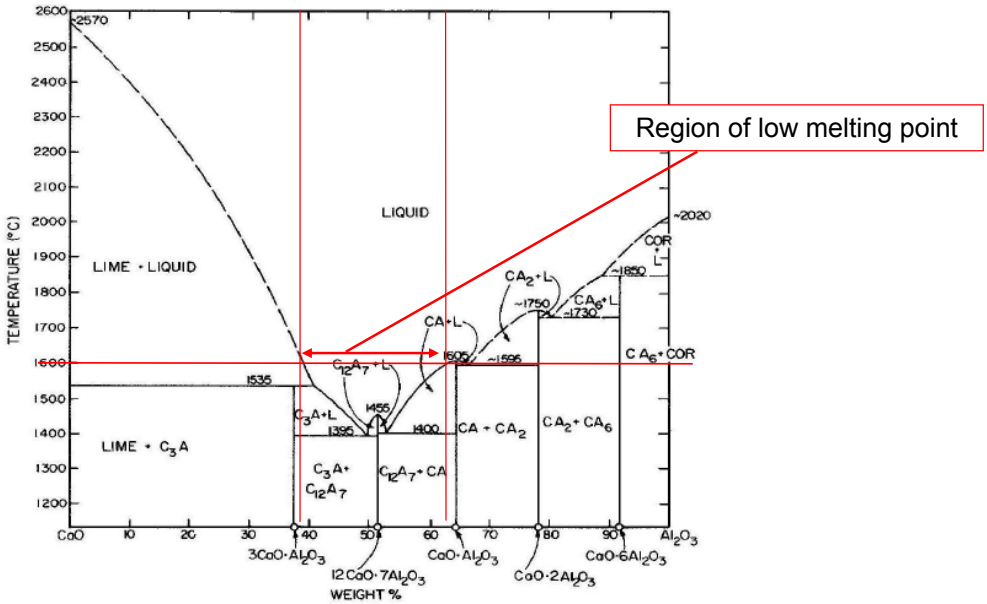
Keith Rackers thesis, 1995

Doloma nozzle



Donald Griffin, LWB, 2007

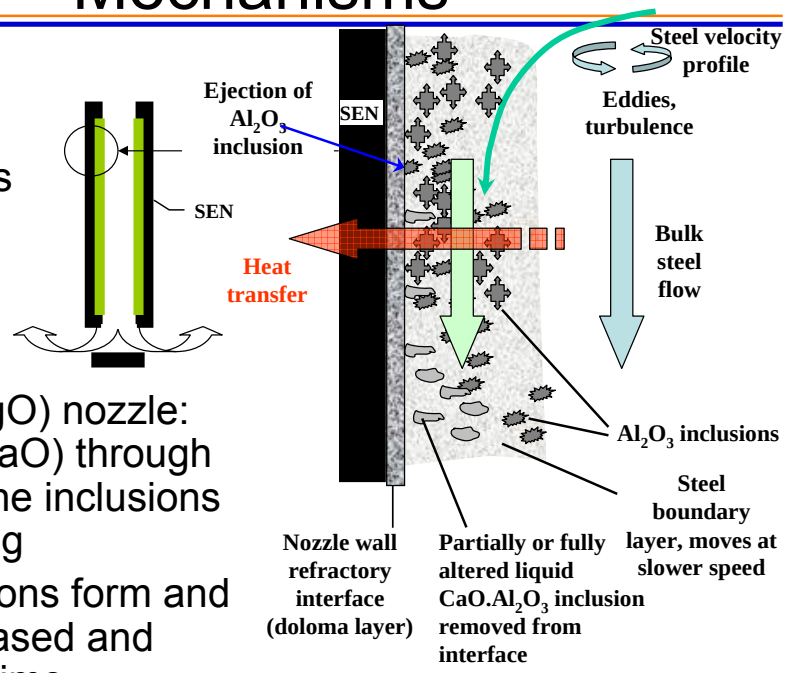
Adding CaO can liquefy Al_3O_3 inclusions



Doloma nozzles utilize this concept to prevent clogging

Nozzle Clogging & Erosion Mechanisms

- Clogging: solid alumina (Al_2O_3) inclusion particles in the steel flow come in contact with nozzle walls
- Doloma (CaO-MgO) nozzle: diffuses calcia (CaO) through nozzle to liquify the inclusions & prevent clogging
- Liquid layers/regions form and particles are released and walls erode with time.



LWB refractories

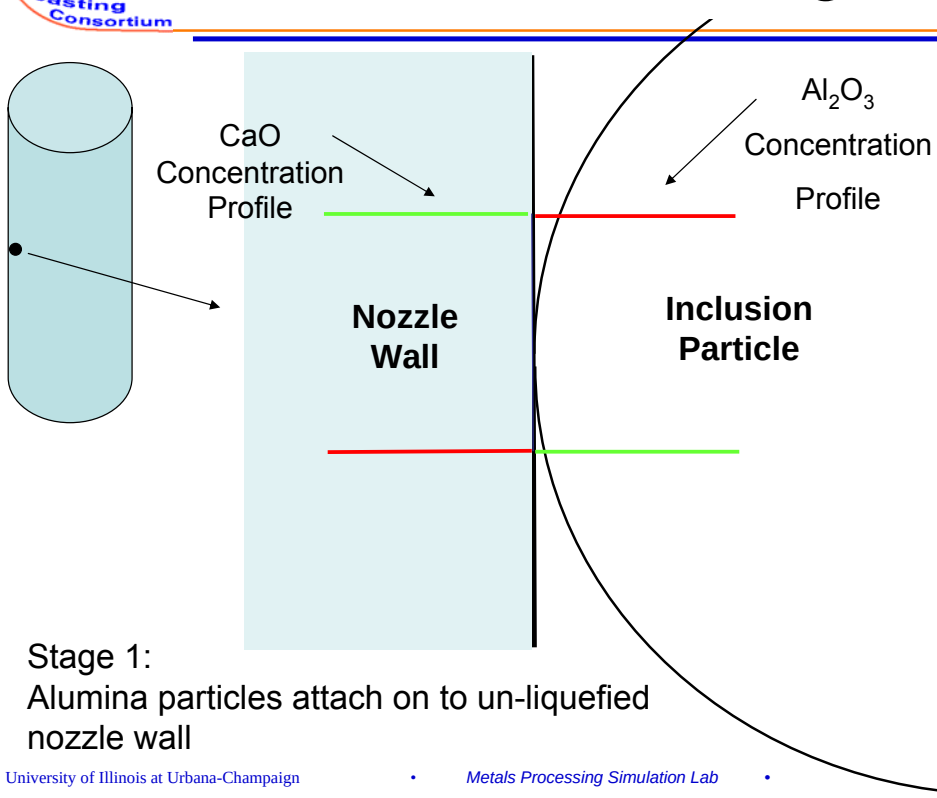
Objectives

- Develop Numerical model (using finite element analysis) to simulate multi-component ion-diffusion, nozzle reactions / phase transformations, erosion, and clogging.
- Use model to predict
  - The dissolution and sweeping away of alumina inclusions
  - Composition of released inclusions
  - Composition evolution and liquefaction of nozzle wall
  - Removal rate of CaO (wall erosion)
  - Particle removal rates

Model Description

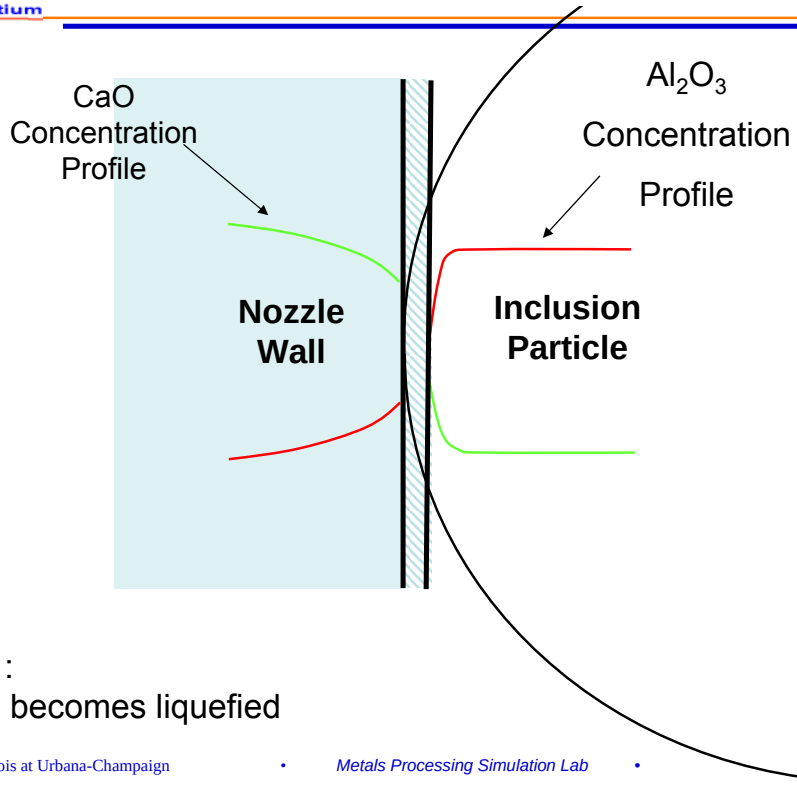
- The nozzle erosion / clogging mechanism will be modeled in 3 microscopic stages:
  - Stage 1: Removal of inclusion particles that touch wall surface, diffuse, partially liquefy, and are carried away, eroding nozzle wall
  - Stage 2: Gradual liquidation of nozzle wall, entrainment of inclusions that touch, and formation of liquid/inclusion matrix layers in the wall
  - Stage 3: Inclusion build up on nozzle surface such that the nozzle wall can no longer liquefy all the inclusions present at the interface.

Nozzle – Stage 1



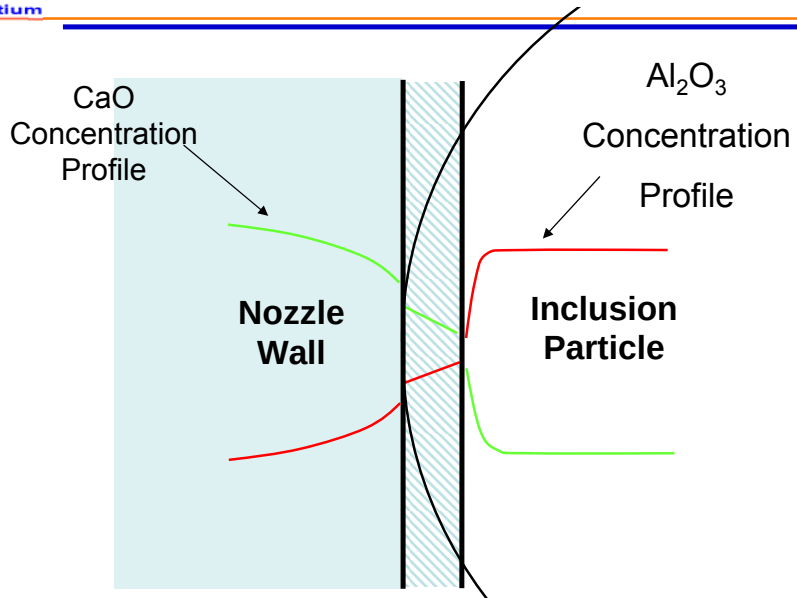
Stage 1:
Alumina particles attach on to un-liquefied nozzle wall

Nozzle – Stage 1



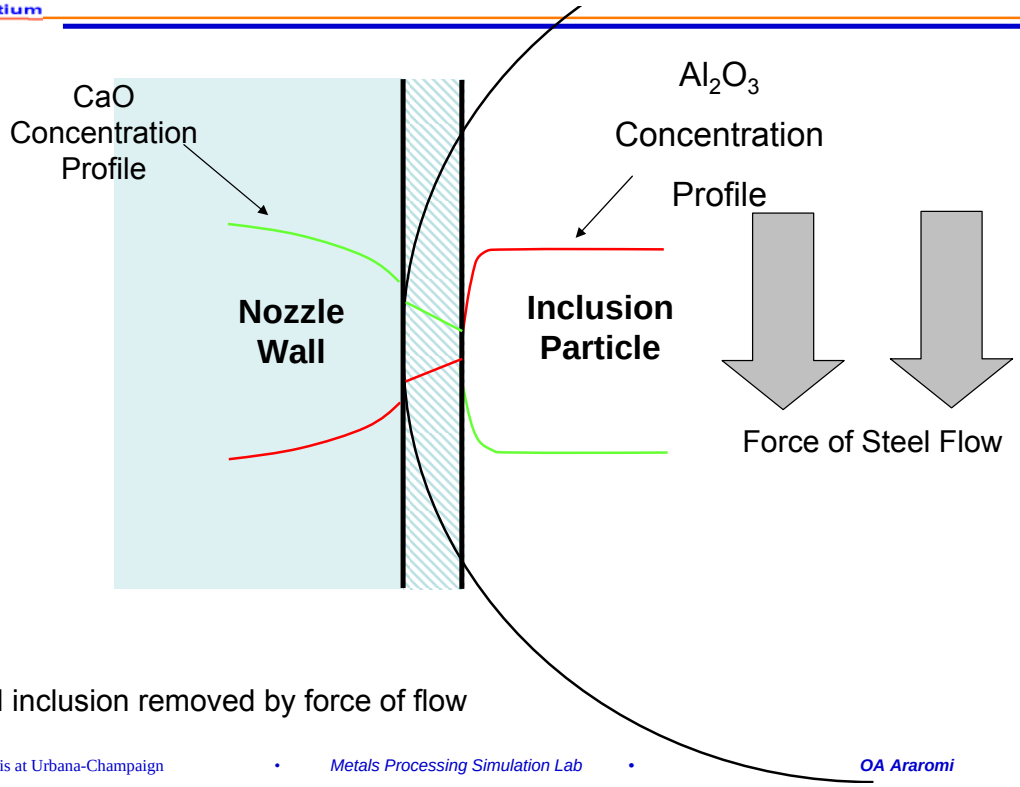
Stage 1:
Particle becomes liquefied

Nozzle – Stage 1



Stage 1:
Particle becomes liquefied

Nozzle – Stage 1

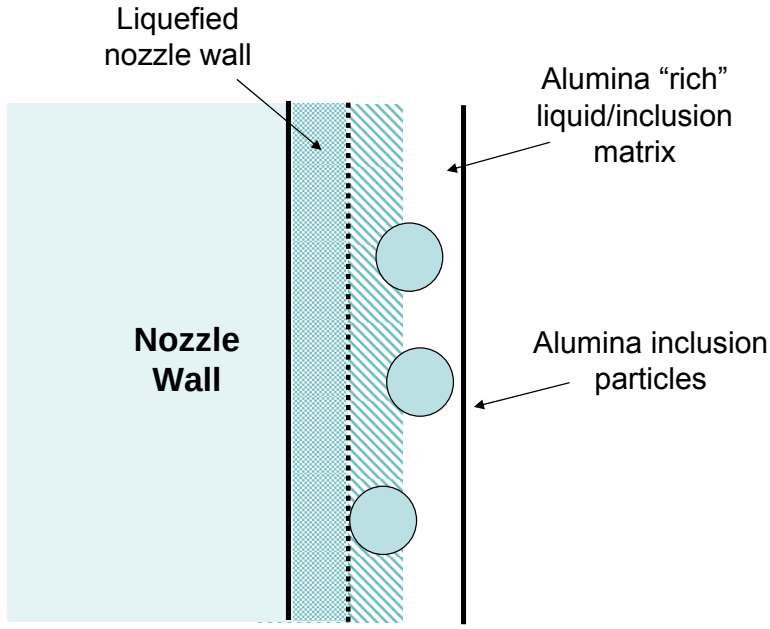


Stage 1:
Liquefied inclusion removed by force of flow

Nozzle – Stage 2

Stage 2:

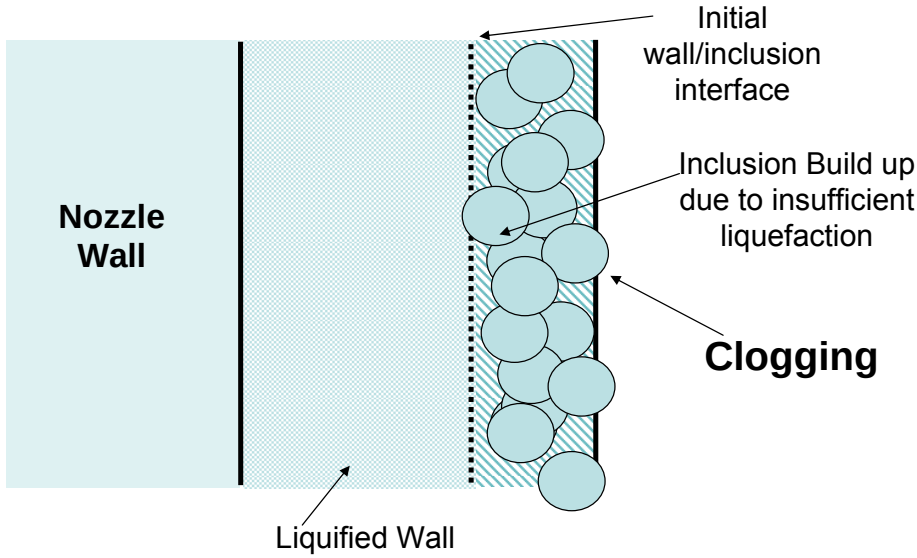
- Nozzle wall becomes liquefied
- Particles stick to liquid wall, form liquid/inclusion matrix
- Inclusions still liquefied (i.e. no solidification)



Nozzle – Stage 3

Stage 3

- Inclusions build up on nozzle wall preventing further liquefaction
- As a result, solidification of the liquid/inclusion matrix can take place.

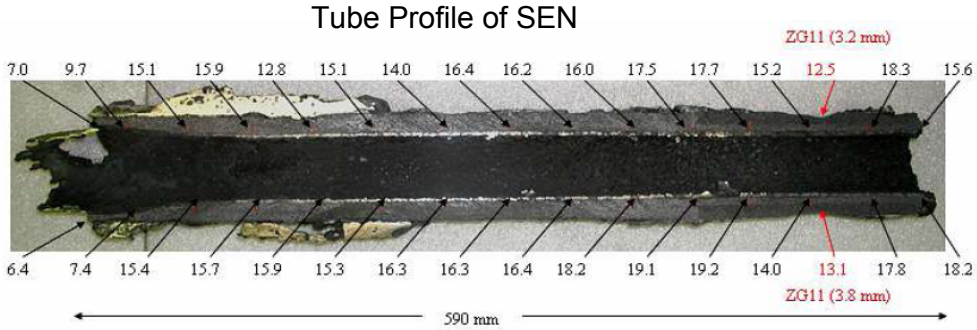


Used Nozzles

Casting time = 191 minutes

Doloma Graphite SEN

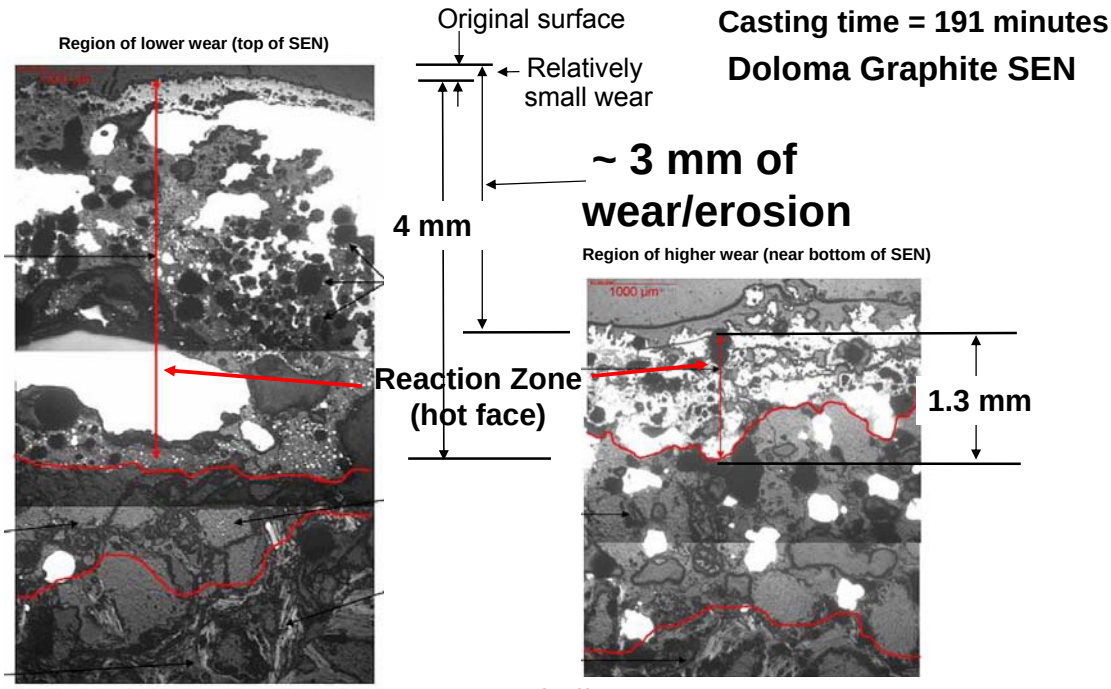
Tube Profile of SEN



- Original thickness ~ 20 mm
- Measurements taken at 50 mm intervals

Donald Griffin, Rob Nunnington LWB , 2007

Nozzle wall microstructure



Donald Griffin, Rob Nunnington, LWB , 2007

Modeling Assumptions

- Diffusion equation is solved for activity
- Assume activity = concentration everywhere in the domain
- Diffusion based on Al_2O_3 concentration, assumed to govern the diffusion process due to low diffusivity
- 1-D assumption (3-D inclusion effects incorporated)
- Assume inclusion particle is initially 100% Al_2O_3
- Assume semi infinite mediums (particle not fully liquid upon release)
- Assume only CaO and Al_2O_3 move by diffusion
- Effects of steel flow not included
- Only MgO and CaO present in new nozzle wall
- Only 3 phase's considered: Al_2O_3 "rich" (solid), CaO "rich" (solid) and liquid with associated diffusion coefficients
- Temperature gradients ignored across the domain
- Concentration on weight basis

Previous Work

- Roy Maske's 1-D model of $CaO\text{-}Al_2O_3$ diffusion couple which used analytical approach to solve diffusion equations
- Analytical equations are limited in their ability to model other effects such as MgO content, etc.

Finite Element Equations

- 1-D diffusion equation

$$\frac{\partial C_\alpha}{\partial t} = \frac{\partial}{\partial x}\left(D_\alpha \frac{\partial C_\alpha}{\partial x} \right)$$

Where: D, is the diffusivity of phase α

C, Concentration of a particular specie in phase α

dx, is the nodal spacing

dt, is the time step

Finite Element Equations

- Galerkin Finite Element Equation (analogous with heat transfer):

$$[C]\{\dot{C}_\alpha\} + [k]\{C_\alpha\} = \{F\}$$

$$\{\dot{C}_\alpha\} = \frac{\{C_{\alpha\,new}\} - \{C_{\alpha\,old}\}}{\Delta t}$$

$$\{C_\alpha\} = \theta\{C_{\alpha\,new}\} + (1-\theta)\{C_{\alpha\,old}\}$$ θ determines the time-step method.

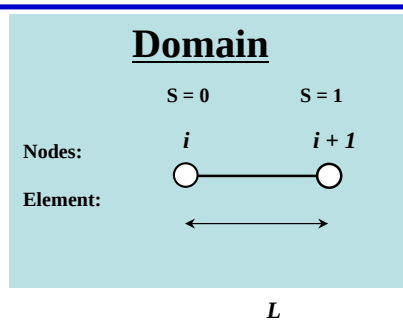
$$[k] = \sum \int_V [B]^T [D][B] dV$$ Diffusivity Matrix

$$[C] = \int_V [N]^T [N] dV$$ Capacitance matrix

$$[F] = \sum \int_V [N]^T V dV$$ Force matrix

$$[D] = D_\alpha$$

Finite Element Equations



s, local co-ordinate system

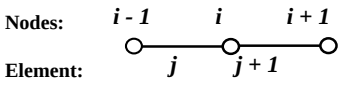
$$\begin{bmatrix} 1-\frac{s}{L} & \frac{s}{L} \end{bmatrix}$$ Shape Function(N)

$$[C_j] = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix} A_j L_j$$ Lumped capacitance matrix

$$[k] = \int_V \begin{bmatrix} -\frac{1}{L} \\ \frac{1}{L} \end{bmatrix} D_\alpha^j \begin{bmatrix} -\frac{1}{L} & \frac{1}{L} \end{bmatrix} dV = \frac{A_j D_\alpha^j}{L_j} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$ Diffusivity matrix

Finite Element Equations

- 2 Element domain



$$[C_j] = \begin{bmatrix} \frac{1}{2}A_jL_j & 0 & 0 \\ 0 & \frac{1}{2}A_jL_j + \frac{1}{2}A_{j+1}L_{j+1} & 0 \\ 0 & 0 & \frac{1}{2}A_{j+1}L_{j+1} \end{bmatrix}$$

$$[k] = \begin{bmatrix} \frac{A_jD_\alpha^j}{L_j} & -\frac{A_jD_\alpha^j}{L_j} & 0 \\ -\frac{A_jD_\alpha^j}{L_j} & \frac{A_jD_\alpha^j}{L_j} + \frac{A_{j+1}D_\alpha^{j+1}}{L_{j+1}} & -\frac{A_{j+1}D_\alpha^{j+1}}{L_{j+1}} \\ 0 & -\frac{A_{j+1}D_\alpha^{j+1}}{L_{j+1}} & \frac{A_{j+1}D_\alpha^{j+1}}{L_{j+1}} \end{bmatrix}$$

From Galerkin Equation

$$\frac{1}{\Delta t}\begin{bmatrix} \frac{1}{2}(AL)_j & 0 & 0 \\ 0 & \frac{1}{2}\left((AL)_j + (AL)_{j+1}\right) & 0 \\ 0 & 0 & \frac{1}{2}(AL)_{j+1} \end{bmatrix}\left\{\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{new}^{\alpha} - \begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{old}^{\alpha}\right\} +$$

$$\begin{bmatrix} \left(\frac{AD_\alpha}{L}\right)_j & -\left(\frac{AD_\alpha}{L}\right)_j & 0 \\ -\left(\frac{AD_\alpha}{L}\right)_j & \left(\frac{AD_\alpha}{L}\right)_j + \left(\frac{AD_\alpha}{L}\right)_{j+1} & -\left(\frac{AD_\alpha}{L}\right)_{j+1} \\ 0 & -\left(\frac{AD_\alpha}{L}\right)_{j+1} & \left(\frac{AD_\alpha}{L}\right)_{j+1} \end{bmatrix}\left\{\theta\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{new}^{\alpha} + (1-\theta)\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{old}^{\alpha}\right\} = \{F\} \cancel{\to} 0$$

Finite Element Equations

- Re-arrange in terms of concentration at current time step

$$\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{new}^{\alpha} = \Delta t[C]^{-1}\left(\frac{1}{\Delta t}[C] - [k]\right)\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{old}^{\alpha}$$

$$\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{new}^{\alpha} = \Delta t\begin{bmatrix} \frac{2}{(AL)_j} & 0 & 0 \\ 0 & \frac{2}{\left((AL)_j + (AL)_{j+1}\right)} & 0 \\ 0 & 0 & \frac{2}{(AL)_{j+1}} \end{bmatrix}\begin{bmatrix} \frac{1}{2\Delta t}(AL)_j - \left(\frac{AD_\alpha}{L}\right)_j & +\left(\frac{AD_\alpha}{L}\right)_j & 0 \\ +\left(\frac{AD_\alpha}{L}\right)_j & \frac{1}{2\Delta t}\left((AL)_j + (AL)_{j+1}\right) - \left(\frac{AD_\alpha}{L}\right)_j - \left(\frac{AD_\alpha}{L}\right)_{j+1} & +\left(\frac{AD_\alpha}{L}\right)_{j+1} \\ 0 & +\left(\frac{AD_\alpha}{L}\right)_{j+1} & \frac{1}{2\Delta t}(AL)_{j+1} - \left(\frac{AD_\alpha}{L}\right)_{j+1} \end{bmatrix}\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{old}^{\alpha}$$

Assuming constant area,

$$\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{new}^{\alpha} = \begin{bmatrix} 1-2\beta_j & 2\beta_j & 0 \\ 2\beta_j\left(\frac{L_j}{L_j + L_{j+1}}\right) & 1-2\beta_j\left(\frac{L_j}{L_j + L_{j+1}}\right) - 2\beta_{j+1}\left(\frac{L_{j+1}}{L_j + L_{j+1}}\right) & 2\beta_{j+1}\left(\frac{L_{j+1}}{L_j + L_{j+1}}\right) \\ 0 & 2\beta_{j+1} & 1-2\beta_{j+1} \end{bmatrix}\begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix}_{old}^{\alpha}$$

$$\beta = \frac{D_\alpha \Delta t}{L^2}$$

Finite Element Equations

- Diffusion coefficient based on phase
- Phase based on concentration (nodal property)
- Geometric averaging of Diffusivities used to determine diffusivity of <u>elements</u>

Nodes: ***i*** ***i + 1***

Element: ***j***

$$D^j = \sqrt{D(C^i) \bullet D(C^{i+1})}$$

Finite Element Equations

Equation for LEFT most node in domain:

$$C_i^\alpha = (1 - 2\beta_j)(C_i^\alpha)_{old} + 2\beta_j (C_{i+1}^\alpha)_{old}$$

Nodes: ***i - 1*** ***i*** ***i + 1***

Element: ***j*** ***j + 1***

Equation for INTERNAL nodes:

$$C_i^\alpha = \beta_j (C_{i-1}^\alpha)_{old} + (1 - \beta_j - \beta_{j+1})(C_i^\alpha)_{old} + \beta_{j+1} (C_{i+1}^\alpha)_{old}$$

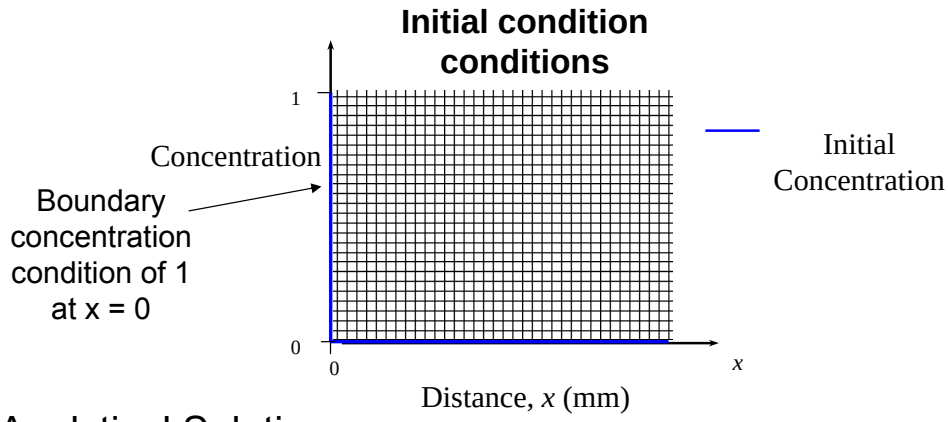
Equation for RIGHT most node in domain:

$$C_i^\alpha = 2\beta_j (C_{i-1}^\alpha)_{old} + (1 - 2\beta_j)(C_i^\alpha)_{old}$$

$$\beta = \frac{D_\alpha \Delta t}{L^2}$$

Model Validation 1

- Finite element solution compared analytical Solution for single species diffusion and single diffusivity

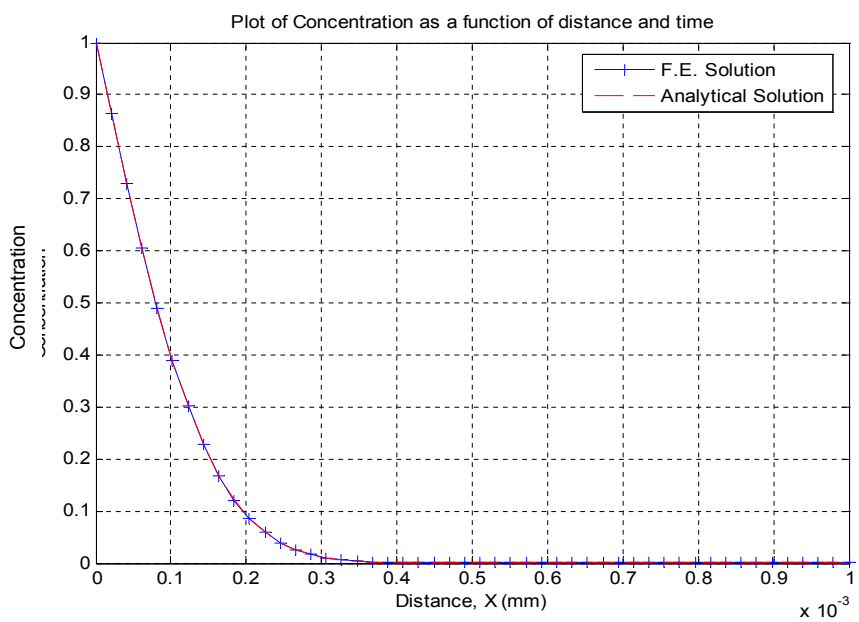


- Analytical Solution,

$$C(x,t) = C_s + erf\left[\frac{x}{2\sqrt{\alpha t}}\right](C_o - C_s)$$

Model Validation 1

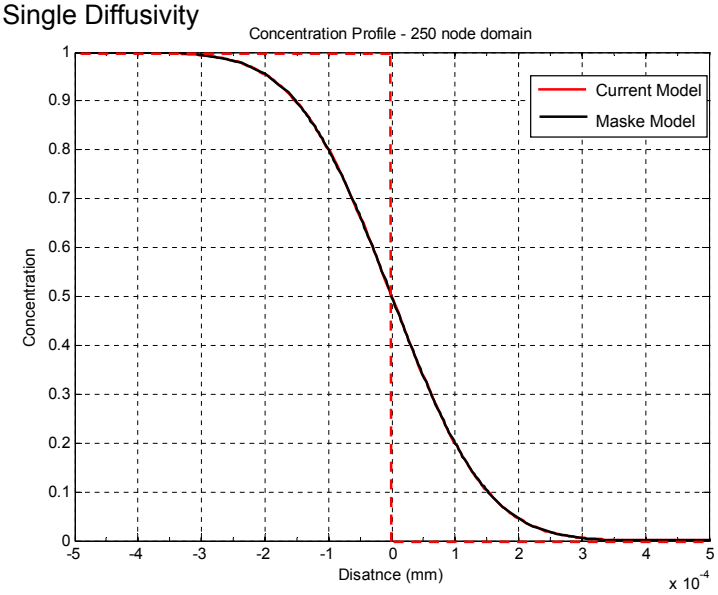
- Solutions match



Model Validation 2

- Validation against previous analytical model:
  - Single diffusion species
  - Single Diffusivity

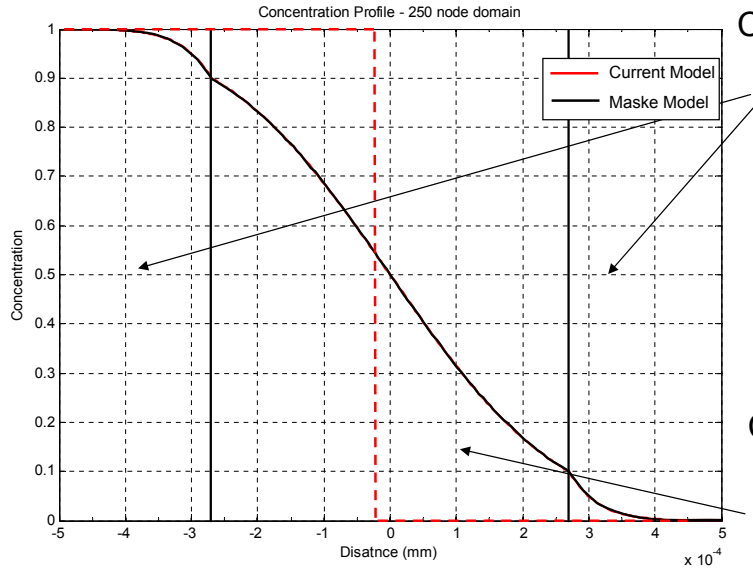
Initial Condition



Model Validation 3

- Validation against previous analytical model:
  - Single diffusion species
  - Multiple Diffusivities (1 order of magnitude difference)

Initial Condition



C > 0.9 or C < 0.1

"Low" diffusion coefficient region (Solid)

C > 0.9 & C < 0.1

"High" diffusion coefficient region (liquid)

Post Processing: to model multicomponent materials

How to find compositions using data from diffusion data of single species?

i.e.

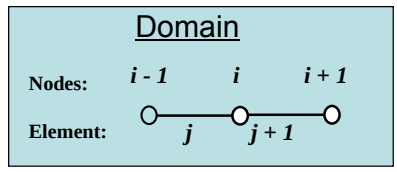
$$\left.\begin{array}{l}\%\ Al_2O_3\\ \%\ CaO\\ \%\ MgO\end{array}\right\}\ \text{Previous time step Composition} \quad + \quad \dot{m}\ \text{(of Al2O3)} \quad \Rightarrow \quad \left.\begin{array}{l}\%\ Al_2O_3\\ \%\ CaO\\ \%\ MgO\end{array}\right\}\ \text{Current time step Composition}$$

Post Processing – mass flows

- Find mass flow rate, $\dot{m}$

From Finite element equations:

$$\begin{bmatrix} B_j & -B_j & \\ -B_j & B_j + B_{j+1} & -B_{j+1} \\ & -B_{j+1} & B_{j+1} \end{bmatrix} \begin{bmatrix} C_{i-1} \\ C_i \\ C_{i+1} \end{bmatrix} = \begin{bmatrix} \dot{V}_{i-1} \\ \dot{V}_i \\ \dot{V}_{i+1} \end{bmatrix}$$



Where; C = Concentration as a result of diffusion equations at current time step

$\dot{V} =$ Volume flow rate (mm³/s)

$$B = \frac{AD}{L}$$

Hence, for Node *i*:

$$\dot{m} = \dot{V} \times \rho_{mix}$$

$$\boxed{\dot{m} = \rho_{mix}\left[-(B_j)C_{i-1} + (B_j + B_{j+1})C_i - (B_{j+1})C_{i+1}\right]}$$

$\rho_{mix} =$ Mixture Density (kg/mm³)

NB: +ve flowing into a node

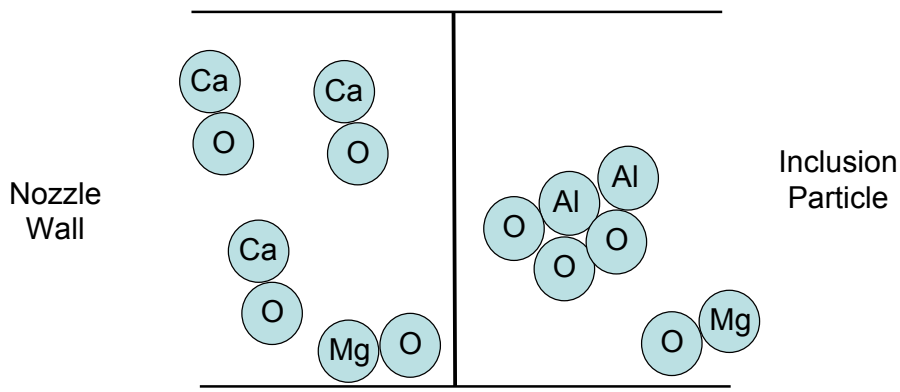
$$\left(\rho_{mix} = \left[\sum_{n=1}^{n} \frac{C_n}{\rho_n}\right]^{-1}, \text{for } n \text{ species}\right)$$

Post Processing - Criterion: charge balance

Diffusion of ceramics is ionic diffusion, charge balance conserved. Net diffusion governed by slower-diffusing atoms

Molar Basis

$$2\,Al(kmol)^{+3} \Leftrightarrow 3\,Ca(kmol)^{+2}$$



Assume Oxygen and Magnesium atoms have no net diffusion

Post Processing – mass ratio calculation

- Charge balance converted to mass ratio

Mass Basis

$$2Al^{+3}(kmol)\times M_{Al}(kg/kmol) \Leftrightarrow 3Ca^{+2}(kmol)\times M_{Ca}(kg/kmol)$$

$$Al^{+3}(kg) = Ca^{+2}(kg)\frac{3M_{Ca}}{2M_{Al}}$$

where; M_{Ca} = 40.08 kg/kmol M_{Al} = 26.98 kg/kmol

- Hence, mass flow rate of Ca found as a function of mass flow rate of Al.

$$\dot{m}_{Ca} = \dot{m}_{Al}\left(\frac{2\times 26.98}{3\times 40.08}\right) = \dot{m}_{Al}\times 2.228$$

Post Processing – new species composition calculation

- New Composition for species *n*

$$\text{Concentration}_n^{New} = \frac{\text{Nodal mass}^{Old} + (\text{mass flow rate}_n \times dt)}{\text{Nodal mass}^{New}}$$

Where,

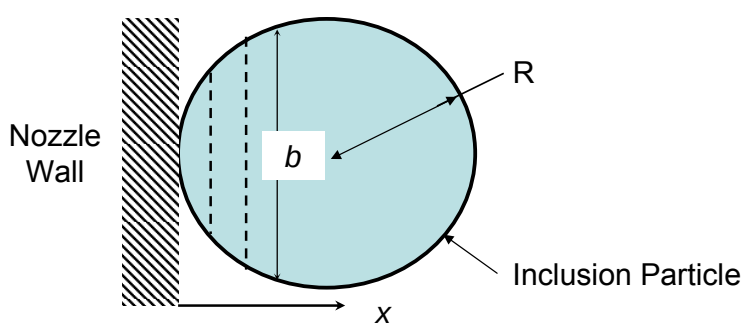
dt = Time step size in seconds

$\text{Nodal mass}^{New} = \text{Nodal mass}^{Old} + (\text{mass flow rate}_{Ca} + \text{mass flow rate}_{Al}) \times dt$

'Old' = previous time step *'New'* = current time step

Spherical Assumption

- model single inclusion as a sphere

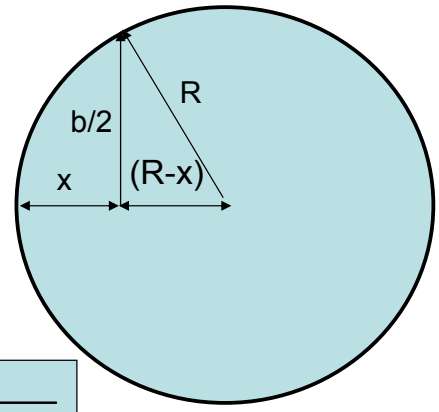


- **The normal length, *b*, can be determine as a function of the distance *x* away from the sphere boundary, and the radius, *R*, of the sphere**

Spherical Assumption

- By geometry:

$$\left(\frac{b}{2}\right)^2 + (R-x)^2 = R^2$$

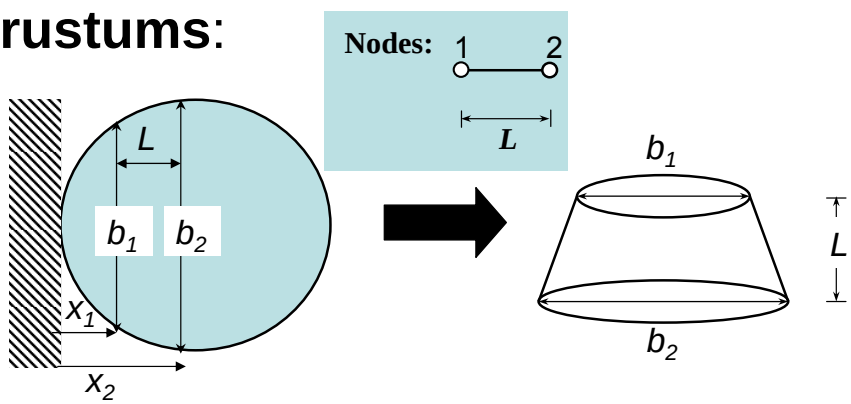


Hence,

$$b = 2 \times \sqrt{R^2 - (R-x)^2}$$

Spherical Assumption

- **Approximate sphere as a series of frustums**:

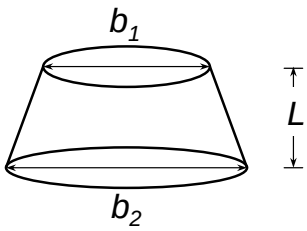


$$b_1 = 2 \times \sqrt{R^2 - (R-x_1)^2}$$

$$b_2 = 2 \times \sqrt{R^2 - (R-x_2)^2}$$

Spherical Assumption

- **Volume of frustums:**



$$Volume = \frac{\pi L}{12}\left(b_1^{\,2} + b_1 b_2 + b_2^{\,2}\right)$$

$$L = (x_2 - x_1)$$

$$Volume = \frac{\pi (x_2 - x_1)}{12}\left(b_1^{\,2} + b_1 b_2 + b_2^{\,2}\right)$$

- **Area,**

$$Area = \frac{\pi}{12}\left(b_1^{\,2} + b_1 b_2 + b_2^{\,2}\right)$$

Choosing Diffusivities

- Published diffusion coefficients vary substantially

Up to 6 orders of Magnitude Difference

Diffusivities in solids and liquid slags

Species	D_0, $cm^2 s^{-1}$	E_D, kcal	Temp range, C	D, $cm^2 s^{-1}$	Temp, K	Temp, C	Oxide/slag	Reference
MgO	-	-		7.90E-05	1823	1550	36CaO/21Al2O3/42SiO2	CMU research
O			1450-1700	3.00E-15	1873	1600	pure solid Al2O3	EPSRC/ Robin Grimes
O			1450-1700	3.00E-17	1773	1500	Pure solid Al2O3	EPSRC/ Robin Grimes
O	167.2	80.7	850-1000	2.34E-12	1273	1000	Pure solid Al2O3	R.G. REDDY, X. WEN, and I.C.I. OKAFOR, MTB VOLUME 31A, DECEMBER 2000
O	1930	152.0	1200-1800	3.54E-16	1773	1500	Single xal Al2O3	Y. Oishi andW.D. Kingery: J. Chem. Phys., 1960, vol. 33, pp. 480-86.
O	2.0	110.0	1200-1800	5.52E-14	1773	1500	polycrstalline Al2O3	Y. Oishi andW.D. Kingery: J. Chem. Phys., 1960, vol. 33, pp. 480-86.
O	6800.0	62.0	750-1000	1.91E-10	1000	727	O and Ti interdiffusivity in TiO2	R.G. REDDY, X. WEN, and I.C.I. OKAFOR, MTB VOLUME 32A, MARCH 2001—491
O	2.0E-03	60.0	710-1300	1.55E-16	1000	727	O in TiO2	R. Haul and G. Dumbgen: J. Phys. Chem. Solids, 1965, vol. 26, pp.1-10
O	870.0	55.6	593-760	6.27E-10	1000	727	O in TiO2	J. Unnam, R.N. Shenoy, and R.K. Clark: Oxid. Met., 1986, vol. 26 (3–4), pp. 231-52.
O	0.1800	83.6	1096-1333	4.50E-18	1100	827	O in TiO2	W.D. Kingery, H.K. Bowen, and D.R. Uhlmann: Introduction to Ceramics.
O				1.26E-17	1667	1394	O in pure MgO	Yang and Flynn
O	1.00E-05	54.0		2.20E-12	1773	1500	pure solid NiO	Geiger and Pourier
O	1.00E+11	146.0		[illegible]	1773	1500	pure solid Fe2O3	Geiger and Pourier
Ca				4.90E-06	1773	1500	51CaO/10Al2O3/39SiO2	Multicomponent Diffusion in Molten Slags M.D. DOLAN and R.F. JOHNSTON
Ca				[illegible]	1773	1500	Optical basicity = 0.68	DOLAN, M.D. and JOHNSTON, R.F.
Ca				3.16E-12	1667	1394	Ca in pure MgO	Yang and Flynn
Ca				4.40E-08	1273	1000	Ca in FeOx	Fukuyama, MTB 33B 2002
Ca				2.69E-09	1273	1000	pure solid CoO	Geiger and Pourier
Al2O3				1.00E-12	1853	1580	solid Al2O3	T.B. Braun, J.F.Elliott and M.C. Flemings: MTB, 10B (1979), 171.
Al2O3				[illegible]	1823	1550	16CaO/19.3Al2O3/64.5SiO2	MONAGHAN, B.J., NIGHTINGALE, S.A., CHEN, L., and BROOKS, G.A.
Al2O3				1.60E-06	1853	1580	28CaO/23.7Al2O3/48.3SiO2	MONAGHAN, B.J., NIGHTINGALE, S.A., CHEN, L., and BROOKS, G.A.
Al	4.30E+04	85.1		5.07E-06	1873	1600	43.5CaO/10Al2O3/46.5SiO2	J. Henderson, L. Yang and G. Derge: Trans. Metall. Soc. AIME, 221 (1961), 56.
Al	5.40E+04	60.0		5.40E-03	1873	1600	38.6CaO/20Al2O3/41.4SiO2	J. Henderson, L. Yang and G. Derge: Trans. Metall. Soc. AIME, 221 (1961), 56.

- Partly due to solid vs. liquid diffusion
- Liquid diffusion coefficient highest

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Choosing Diffusivites

- However CaO on average has the highest diffusivity:

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Self diffusion coefficients in liquid pure species and slags (Mills in Sla

Species	D_0, cm²s⁻¹	E_D, kcal	Temp range, C	D, cm²s⁻¹	Temp, K	Temp,
Al	5.37	60.0	1398-1487	1.04E-07	1700	1427
Al	0.0023	21.2	2050-2300	6.58E-06	1823	1550
O	0.0066	10.7	1420-1550	3.44E-04	1823	1550
O	0.0162	16.6	1420-1550	1.65E-04	1823	1550
O	8.3176	22.9	1000-1200	1.85E-03	1373	1100
O	6606934	97.5	1550-1650	2.77E-05	1873	1600
O	12303	87.2	1550-1650	8.15E-05	1873	1600
Ca	22.91	60.0	1420-1515	7.99E-07	1758	1485
Ca	0.71	36.0	1420-1550	2.59E-05	1773	1500
Ca	0.21	31.9	1400-1600	2.44E-05	1773	1500

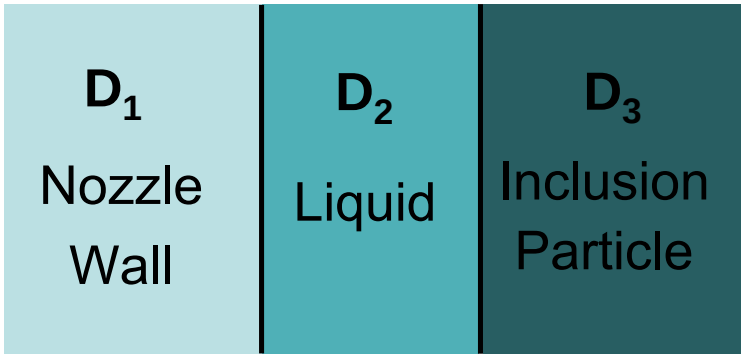
Self diffusion coefficients in liquid slag (Richardson)

Species	D_0, cm²s⁻¹	E_D, kcal	Temp range, C	D, cm²s⁻¹	Temp, C	Slag
Ca	-	38-70	1350-1450	6.70E-07	1400	CAS
	-			4.00E-06	1545	CAS
	-			3.00E-07	1340	40/20/40
	-			1.90E-06	1500	40/20/40
	-	32	1450-1500	5.50E-06	1500	38/20/42
	-	50	1485-1530	7.00E-07	1500	55C/45S
	-		1420-1485	8.00E-07	1500	49C/51A
Si	-	70	1350-1450	1.00E-07	1450	CAS
				2.00E-07	1500	40/20/40
				2.00E-07	1470	40/20/40
	-			3.00E-08	1360	40/20/40
O	4.7	85	1350-1450	6.00E-06	1450	CAS
				1.90E-05	1500	40/20/40
				4.00E-05	1550	40/20/40
	-			2.00E-06	1375	40/20/40
Al				7.00E-07	1480	40/20/40
				2.50E-07	1410	40/20/40
	5.4	60	1400-1520	7.00E-07	1500	44/12/44
Fe	-	40	1250-1305	7.90E-05	1250	61FeO/39SiO2
				1.20E-04	1304	
S				2.70E-06	1580	40/20/40
				8.50E-07	1440	40/20/40

- CaO movement by diffusion "easier" than Al2O3 movement by diffusion
- Hence, calculate Al2O3 diffusion only (model)
- Assume CaO diffuses fast enough to satisfy charge balance, based on local Al2O3 concentration (post processing)

Choosing Diffusivities

- Diffusivities used:
  - **D_1** (CaO "rich" solid) = **1×10^{-6} mm²/s**
  - **D_2** (Liquid-rich) = **5×10^{-4} mm²/s**
  - **D_3** (Al_2O_3 "rich" solid) = **1×10^{-9} mm²/s**

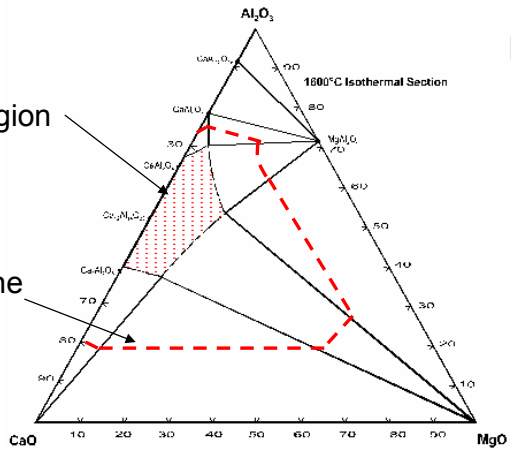


Choosing Diffusivities

- Assume liquid diffusivity, D_2, acts on compositions with 50% liquid and above

100 % liquid region

50 % Liquid line



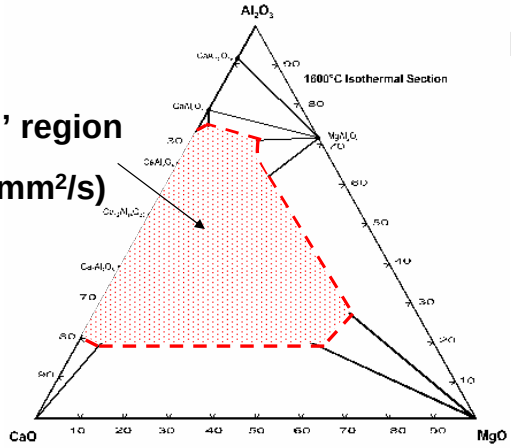
Isotherm section: 1600 C

Choosing Diffusivities

- Assume a single liquid layer and associated diffusion coefficient.

Single 'liquid' region

(D_2 = 5x10^{-4} mm^2/s)



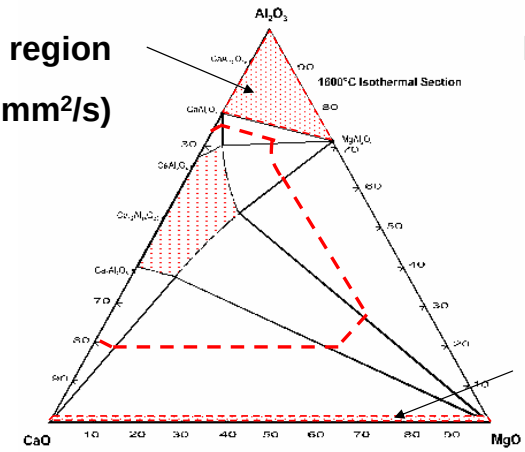
Isotherm section: 1600 C

Choosing Diffusivities

- Single diffusivities for Al2O3 “rich” and CaO “rich” regions

Al_2O_3 “rich” region

(D_3 = 1x10^{-9} mm^2/s)



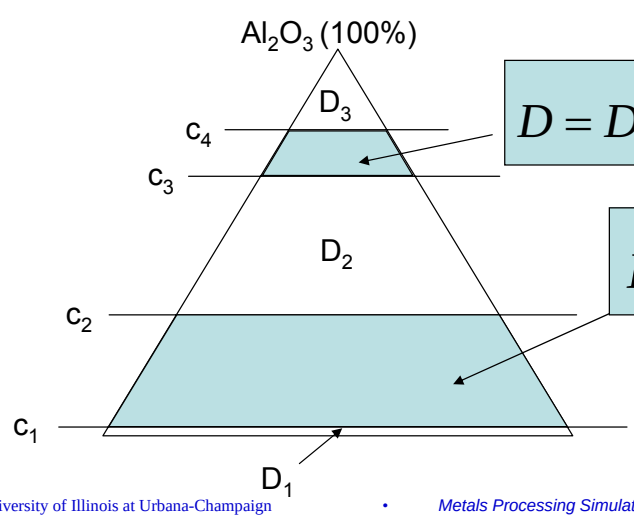
Isotherm section: 1600 C

CaO “rich” region

(D_1 = 1x10^{-6} mm^2/s)

Choosing Diffusivities

Geometric averaging used to determine diffusion coefficients when not in liquid, CaO “rich” or Al_2O_3 “rich” regions



$$D = D_2^{\left(\frac{C-c_1}{c_2-c_1}\right)} \times D_1^{\left(\frac{c_2-C}{c_2-c_1}\right)}$$

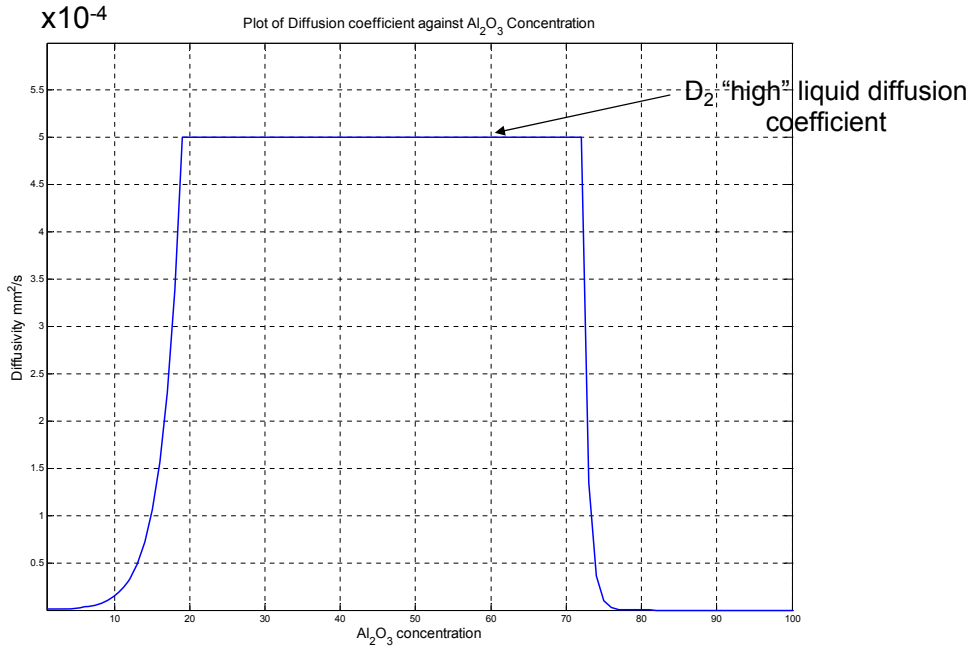
$$D = D_2^{\left(\frac{c_4-C}{c_4-c_3}\right)} \times D_3^{\left(\frac{C-c_3}{c_4-c_3}\right)}$$

C = Al_2O_3 Concentration

c_1 to c_4: Al_2O_3 Boudary Concentrations

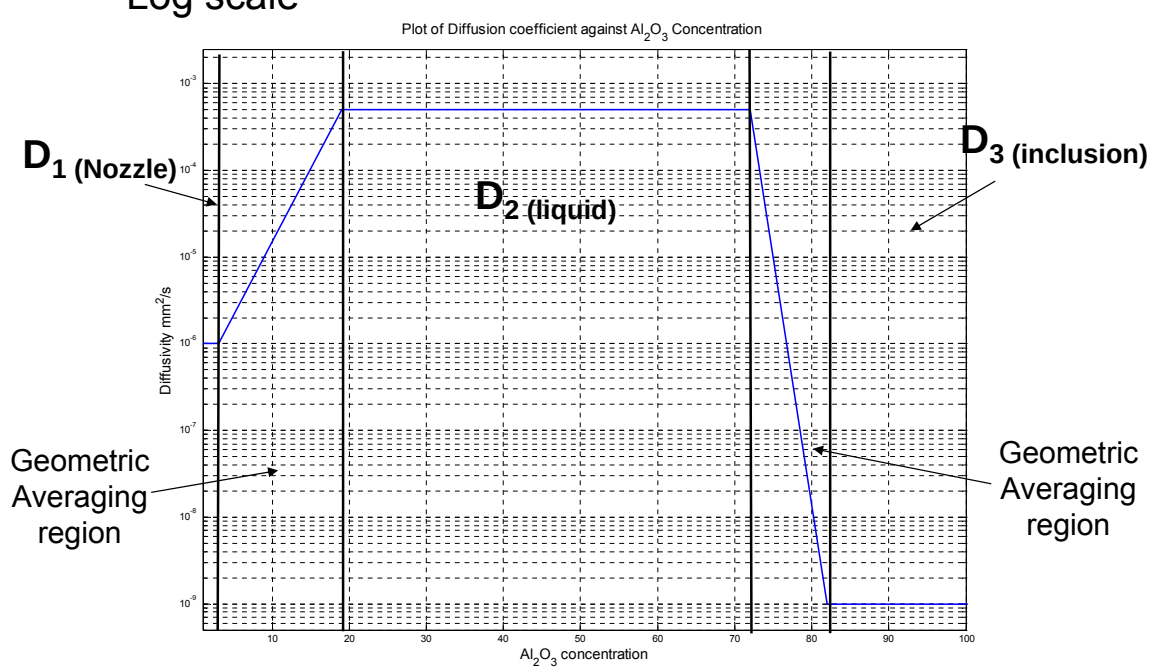
Choosing Diffusivities

Plot of Diffusion coefficient against Al_2O_3 concentration MgO concentration = 10%



Choosing Diffusivities

- Log scale



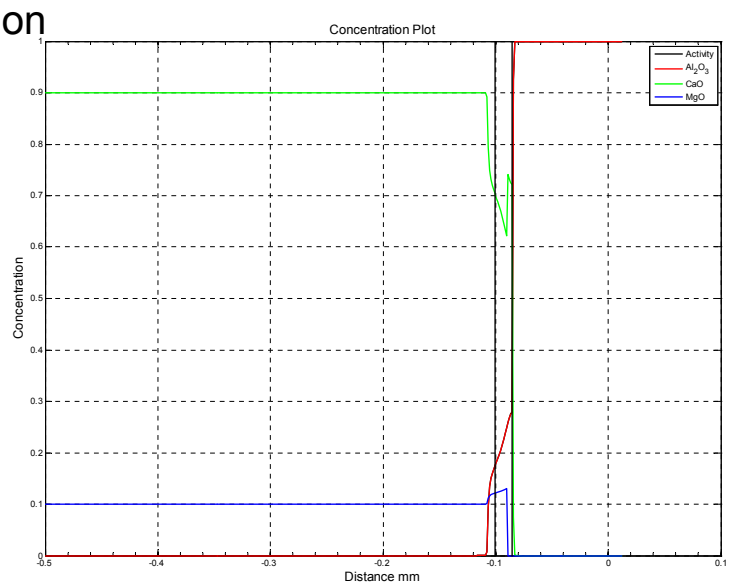
Results – Stage 1

Model Inputs:

- Model inclusion as spherical particle
- Inclusion diameter = 100 microns
- Contact region with nozzle wall = 20 microns diameter (Ratio of max inclusion area to contact area =25:1)
- Initial nozzle wall composition is 90% CaO, 10% MgO
- Critical liquid layer thickness before particle detachment = 20 microns
- All liquid removed with particle
- Removed particle immediately replaced by another
- Temperature 1600 C

Results – Stage 1

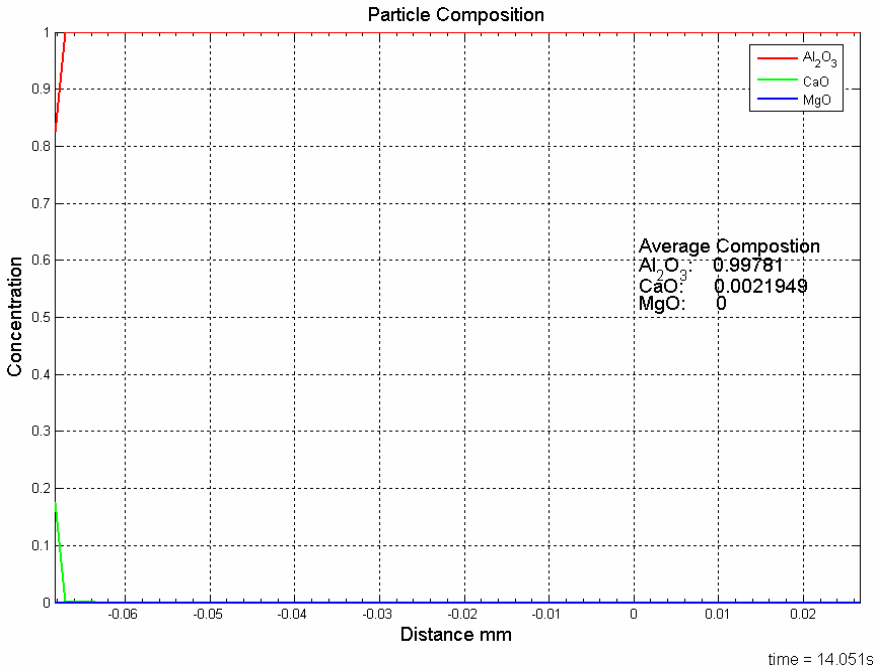
Animation



- First Particle caused wall liquefication
- Hence, mininimum stage 1 duration time is 0 sec

Results – Stage 1

Particle composition



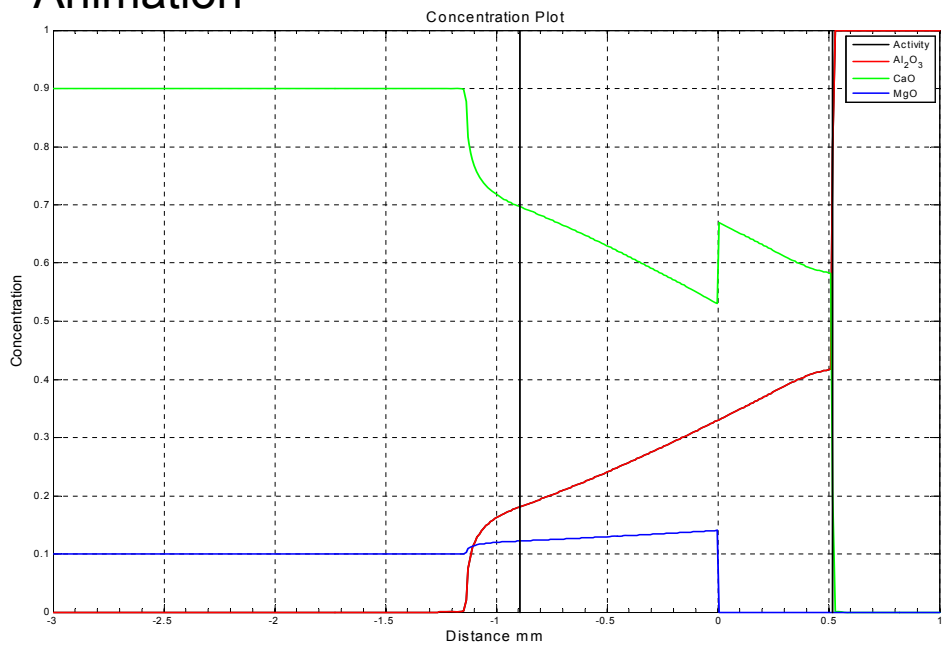
Results – Stage 2

Model Inputs:

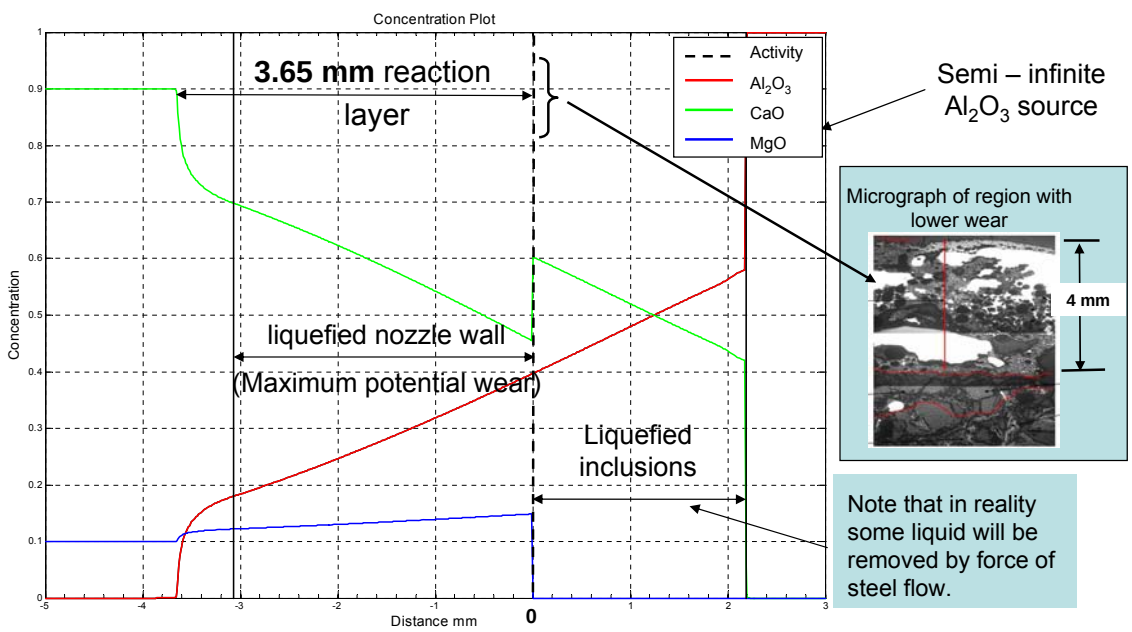
- Initial nozzle wall composition is 90% CaO, 10% MgO
- Al_2O_3 concentration fixed at 100 % on right domain boundary
- No area variation
- Initial nozzle/particle interface a X = 0
- No material removed
- Temperature 1600 C

Results - Stage 2

- Animation

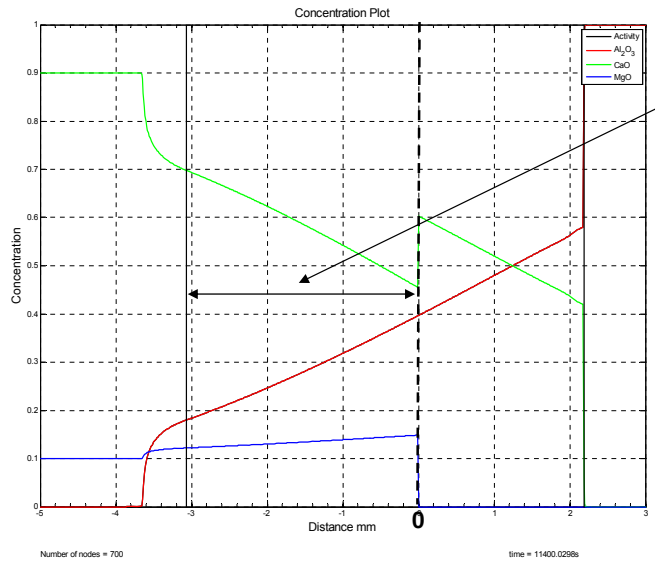


Comparison with used nozzle measurements



Simulation time = 190 mins (11400 sec)

Estimation of CaO removal rate



3.1 mm of wear assuming all liquid is removed (worse case scenario)

The mass removed per unit area is therefore = 3.1 x 3.36×10^{-6} = **1.04×10^{-5} kg/mm²**
(using an approximate wall density = 3.36×10^{-6} kg/mm³)

Mass of CaO removed per unit area = 1.04×10^{5} x 0.9 = **9.4×10^{-6} kg/mm²**

Removal rate of CaO

= (9.4×10^{-6} kg/mm²) / 190 mins

Removal rate of CaO = 4.9×10^{-8} kg/mm² min

Estimation of CaO removal rate

For an SEN surface area = π x 60 x1000 = 1.88×10^{5} mm²

CaO removal rate = 1.88×10^{5} x 4.9×10^{-8} = **9.3×10^{-3} kg/min**

Flow rate of steel = SEN cross-section x flow velocity (1.5 m/s) x steel density (7.0×10^{-6} kg/mm³)

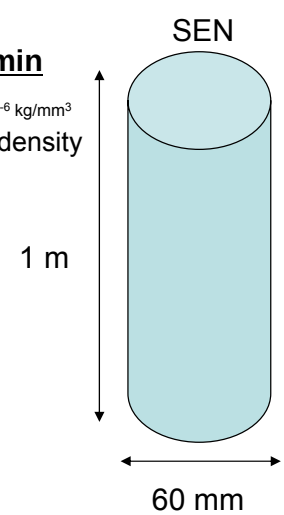
= **1780 kg/min**

Hence,

Max (upper limit) of CaO ppm in steel final product:

= $9.3 \times 10^{-3} / 1780 \times 1 \times 10^{6}$

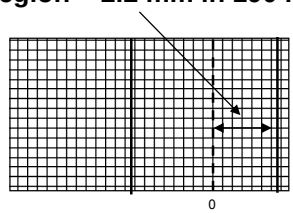
= 5.2 ppm



Estimation of inclusion limit

Can use liquefied inclusion region to estimate an inclusion limit/maximum that the nozzle can handle before clogging can occur:

- Liquefied inclusions region = 2.2 mm in 190 min (~ 3hrs) from previous figure



- Total mass of inclusions per unit area of nozzle as function of time:

= 2.2 x liquid density

(density approx. 3.6 $\times 10^{-6}$ kg/mm3 using average liquid composition)

= 7.92 $\times 10^{-6}$ kg/mm^2
(for time = 190 mins)

or,

Inclusion liquefaction rate = 4.17 $\times 10^{-8}$ kg/mm^2 min

Estimation of Inclusion limits

Assume an average inclusion particle diameter of 100 microns

~ 4 $\times 10^{-6}$ kg/mm^3

Average inclusion mass = 4/3 x π x (50 $\times 10^{-3}$)3 x (density of alumina)

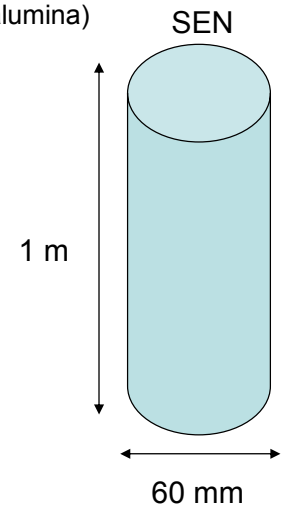
= 2.1 $\times 10^{-9}$ kg

Hence,

Inclusion limit = $\frac{\text{total mass of inclusions per unit area time}}{\text{Average inclusion mass}}$

= $\frac{4.17 \times 10^{-8} \text{ kg/mm}^2 \text{ min}}{2.1 \times 10^{-9} \text{ kg}}$

~ 20 inclusion /mm^2 min



With an SEN with a surface are = 1.88x10^5 mm^2

Inclusion limit = 3.8 million inclusions per min

Estimation of Inclusion limits

- Can express inclusion limit in terms of ppm:

For the SEN dimensions as shown on the previous slide,

Inclusion limit = $1.88 \times 10^{5} \times 4.17 \times 10^{-8}$

= **7.84×10^{-3} kg/min**

Steel flow rate = **1780 kg/min** (as shown on slide 54)

Inclusion limit (ppm) = $7.84 \times 10^{-3} / 1780 \times 10^{6}$

= **4.40 ppm**

(Note: This estimate is conservative, as model assumes a continuous Al_2O_3 source)

Interpreting Results

- Assume:
  - a steel flow rate of 1780 kg/min
  - Steel upstream inclusion content of 40 ppm
  - On average 10% of the inclusions come in contact with nozzle wall (4 ppm)
  - Casting time = 190 mins
- Nozzle walls can liquefy 4.4 ppm inclusions, so should **not** clog in this time

Summary

- 1-D Numerical model of ceramic ion diffusion developed for Al_2O_3 - CaO - MgO refractory systems
- Model tracks the inclusion particle interaction with a nozzle and simulates the stages of inclusion deposition and removal, wall liquefaction and inclusion entrainment and the insufficient liquefaction of inclusions leading to conventional clogging.
- The model provides a frame work for studying composition evolution and the behavior of nozzle/inclusion interactions
- Model results provide estimations of:
  - The removal rate of CaO from doloma nozzle wall
  - The lower limit on the amount of inclusion the nozzle can handle before clogging is likely.
  - The maximum wall erosion

Acknowledgments

- Continuous Casting Consortium Members (Nucor, Postech, LWB Refractories, Algoma, Corus, Labein, Mittal Riverdale, Baosteel, Steel Dynamics)
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