Modelling of High Temperature Processes

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Mathematics Discipline

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High Temperature Processes ?

Materials Production

Cement, Steel, Aluminium, Magnesium, Glass, Ceramics and others

Manufacturing/Fabrication

Casting, Joining, Welding, Heat Treatment and others

Energy Conversion

Combustion and Nuclear

Image from http://www.geokem.com/OIB-volcanic-hawaii.html

Image from www.uksteel.org.uk/stlmake4.htm

What is special about high temperatures ?

Ability to rapidly transform

Often highly reactive and transient systems

Interaction between chemistry and physics

Difficulty of measurement

Challenge to understand and control

Modelling of High Temperature Systems

- The trap of phenomenology
- Using models to “inform” experiments
- Using models to develop theoretical debate
- Using models as predictive tools
- Using models for process control

Modelling of High Temperature Processes

- Computational Thermodynamics – Well Established
- Computational Fluid Dynamics – Well Established
- "Black Box" Process Models (i.e. Neural Networks, Multivariate Statistics etc) – Rapid Development
- Computational Kinetics – Developing

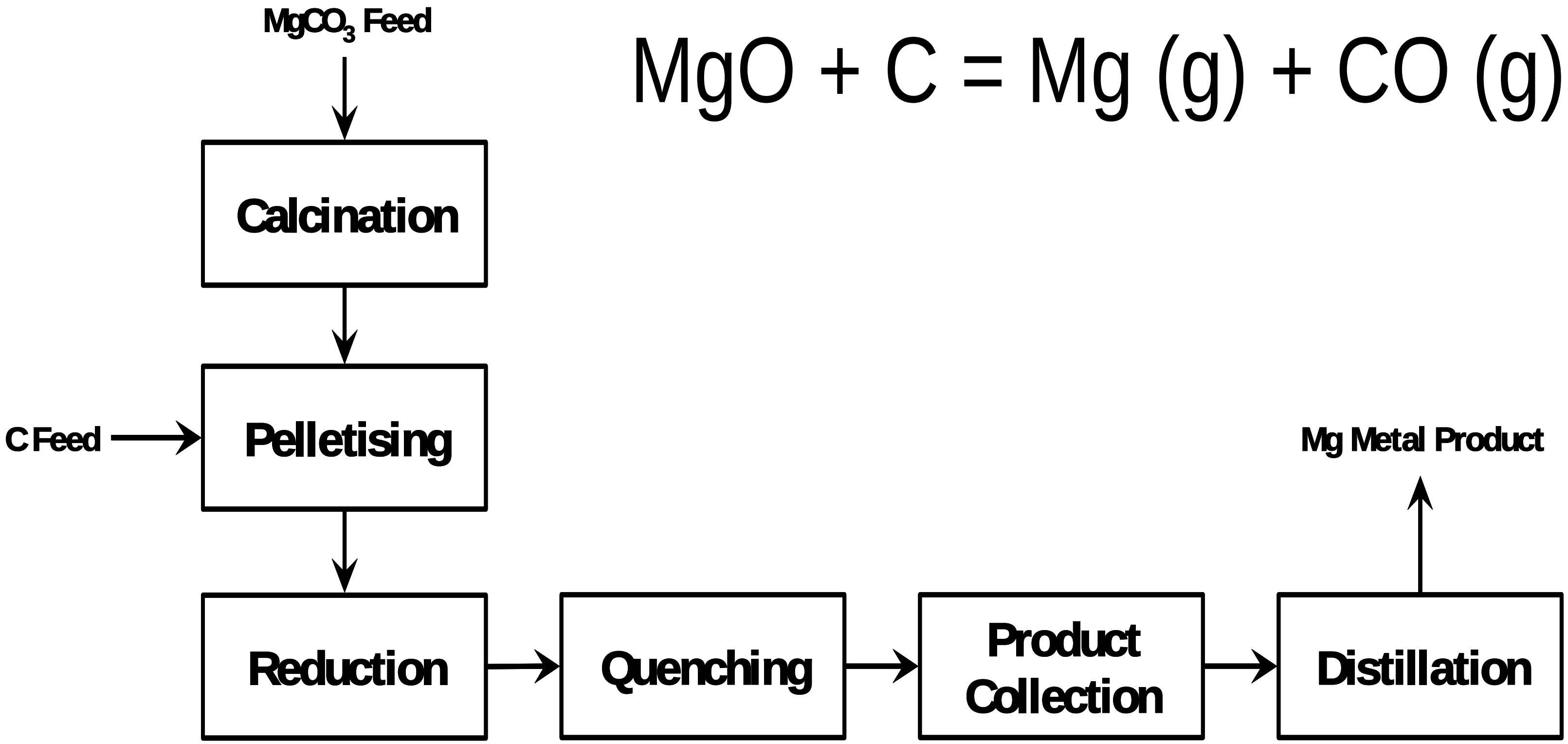
Issues: Coupling with CFD

Multi-scale modelling

Limits of theory (e.g. convective mass transfer)

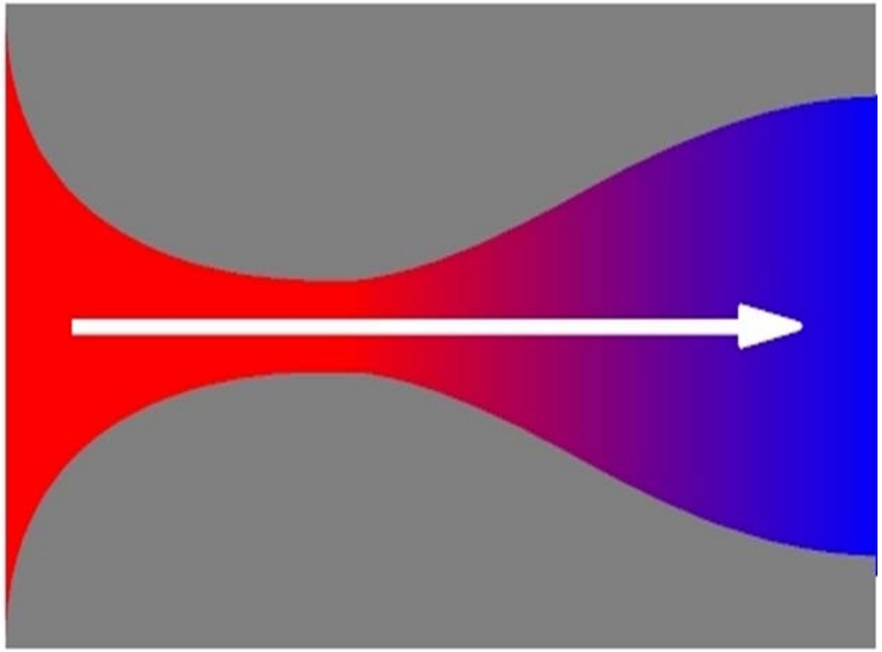
Magnesium Quench Route at CSIRO

$$MgO + C = Mg\ (g) + CO\ (g)$$



Brooks et al., 2007

Adibatic Expansion in Nozzles

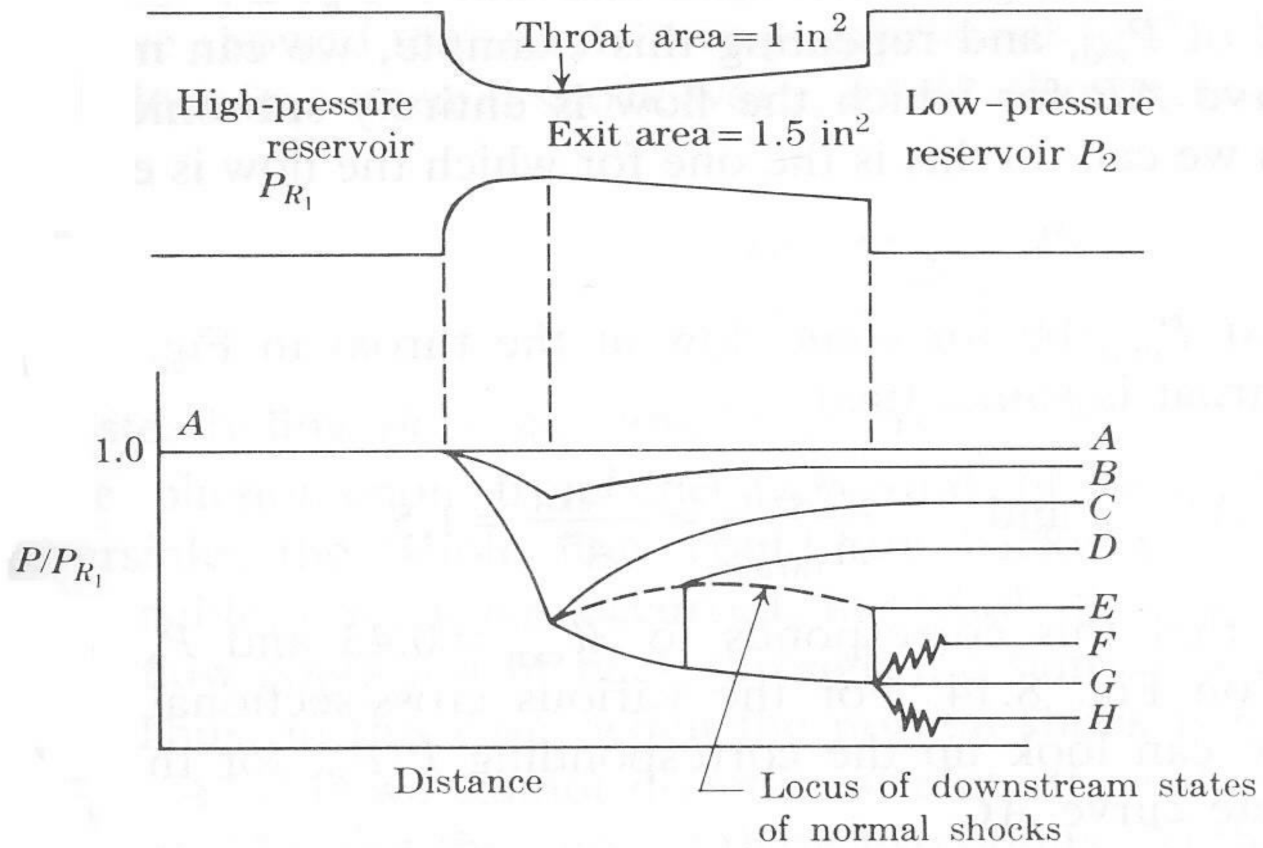


$$\frac{T_1}{T_2} = \frac{(k-1)Ma_2^2 + 2}{(k-1)Ma_1^2 + 2}$$

It is Rocket Science !!

aprl.db.erau.edu/generalinfo/soundingrockets/...

Laval Nozzles



Thermodynamics of System

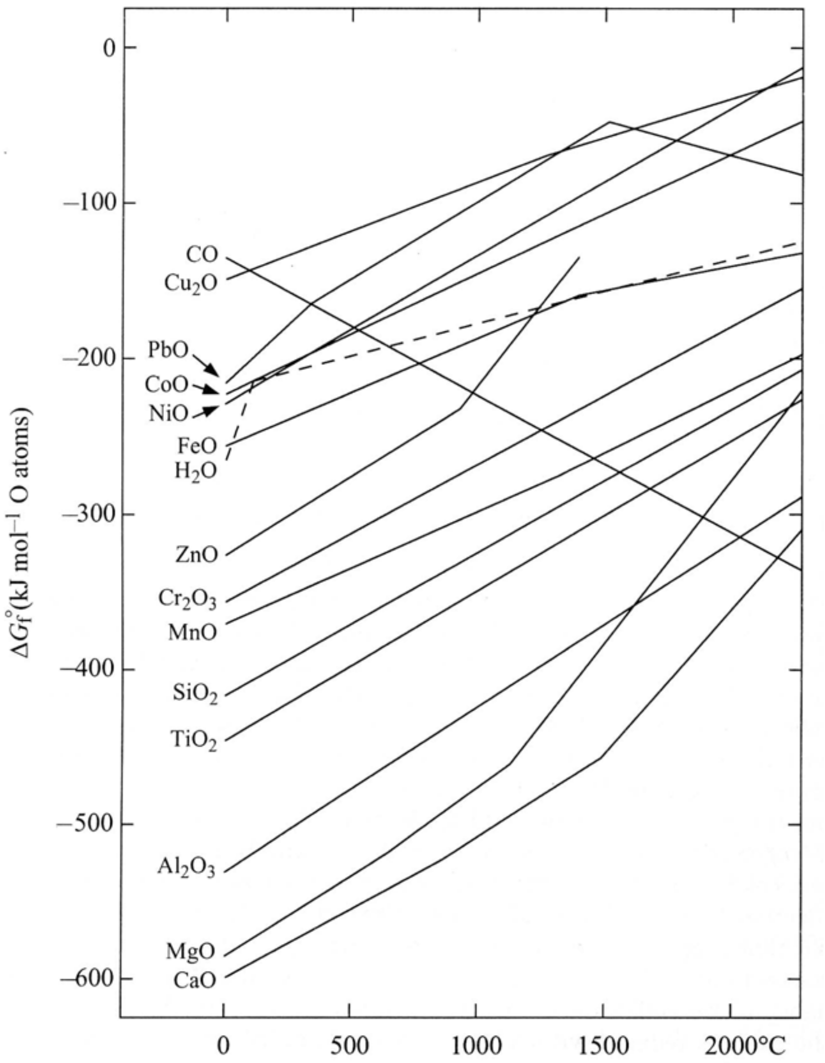


Figure 17.9 Ellingham diagram for formation of several oxides.

- Gibbs energy criteria
- Impurity distribution
- Energy balances
- Development of therm. models
- Challenge of solution behaviour

Image from Swaddle, Inorgnic Chem., 1997

Thermodynamic Modelling

$$nG = \sum_{i=1}^{N} n_i \overline{G}_i$$ = total free of system

$$\sum_{i=1}^{N} n_i a_{ji} = b_j$$ Mass balance restraint

n_i = number of moles of i, N = total number of species,
a_{ji} = number of g atoms of element j b_j = total g atoms of element j

Thermodynamic Modelling

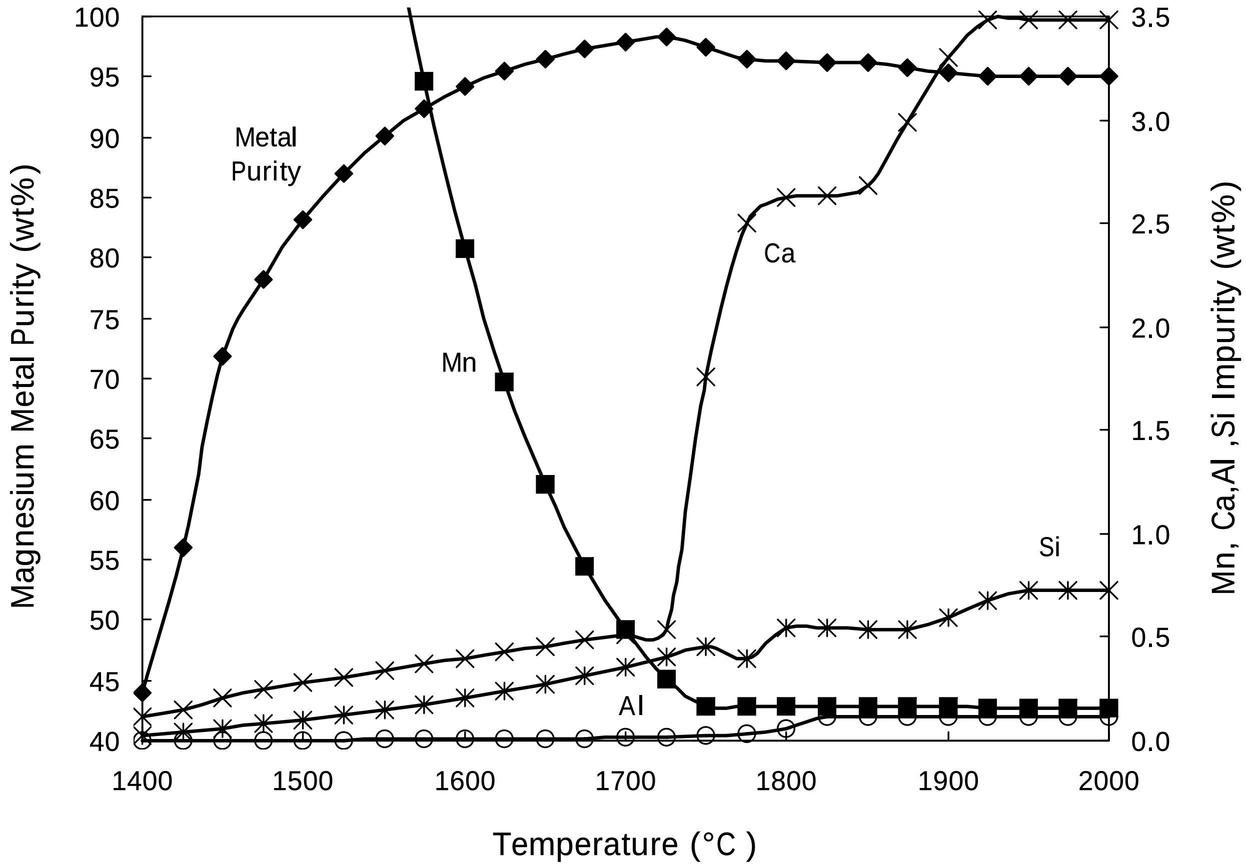
$$\Delta G_i = n_i RT \ln a_i$$

$$a_i = \gamma_i x_i$$ = activity of dissolved species i

γ_i = activity coefficient of i in solution
= f (temperature, conc. of all dissolved species)

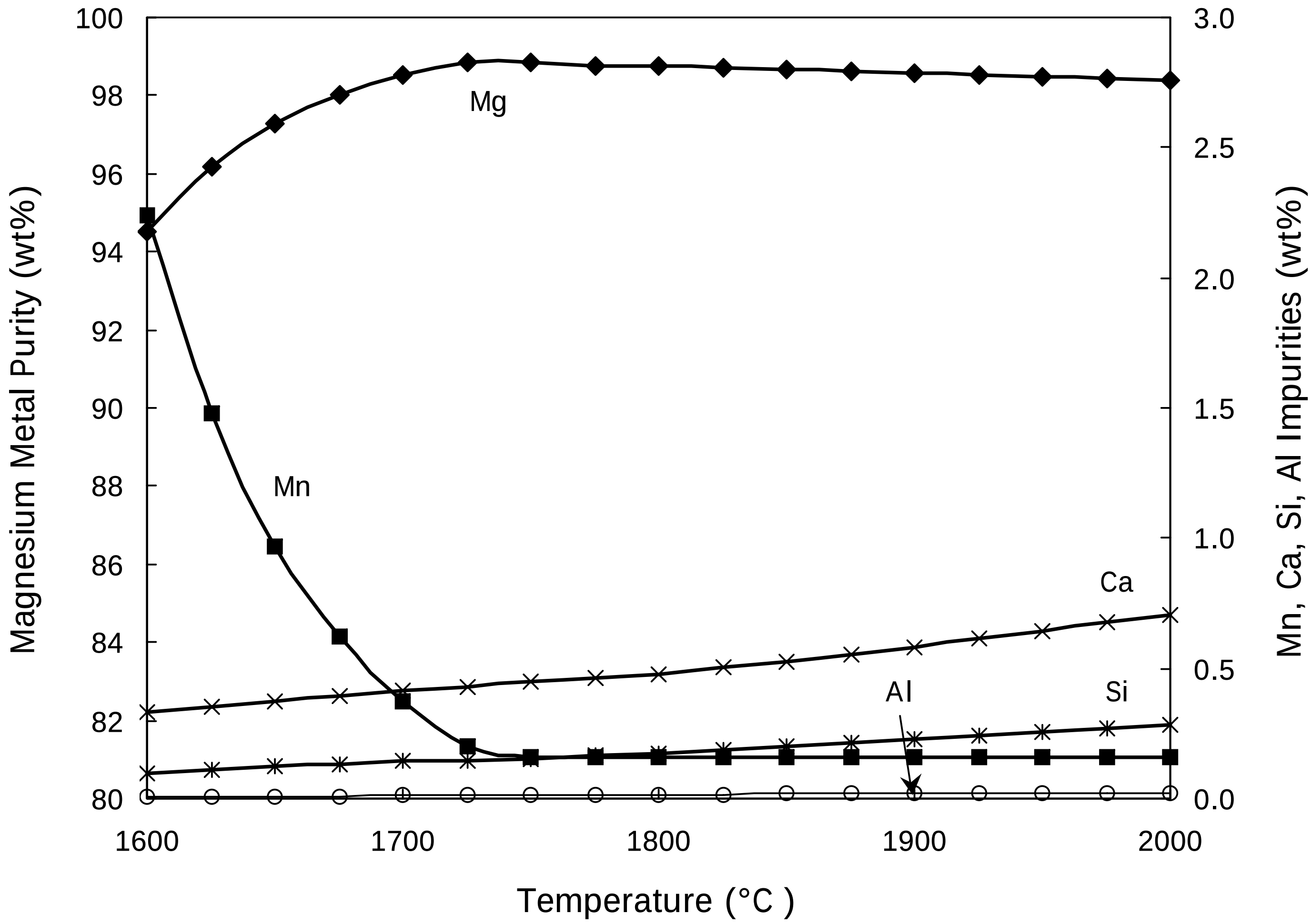
x_i = molar concentration of i in solution
R = Gas constant, T = temperature

Predicted purity of Magnesium – no flux



Brooks et al., The Physical Chemistry of Carbothermic Route to Mg, 2006

Predicted purity of Magnesium – with flux



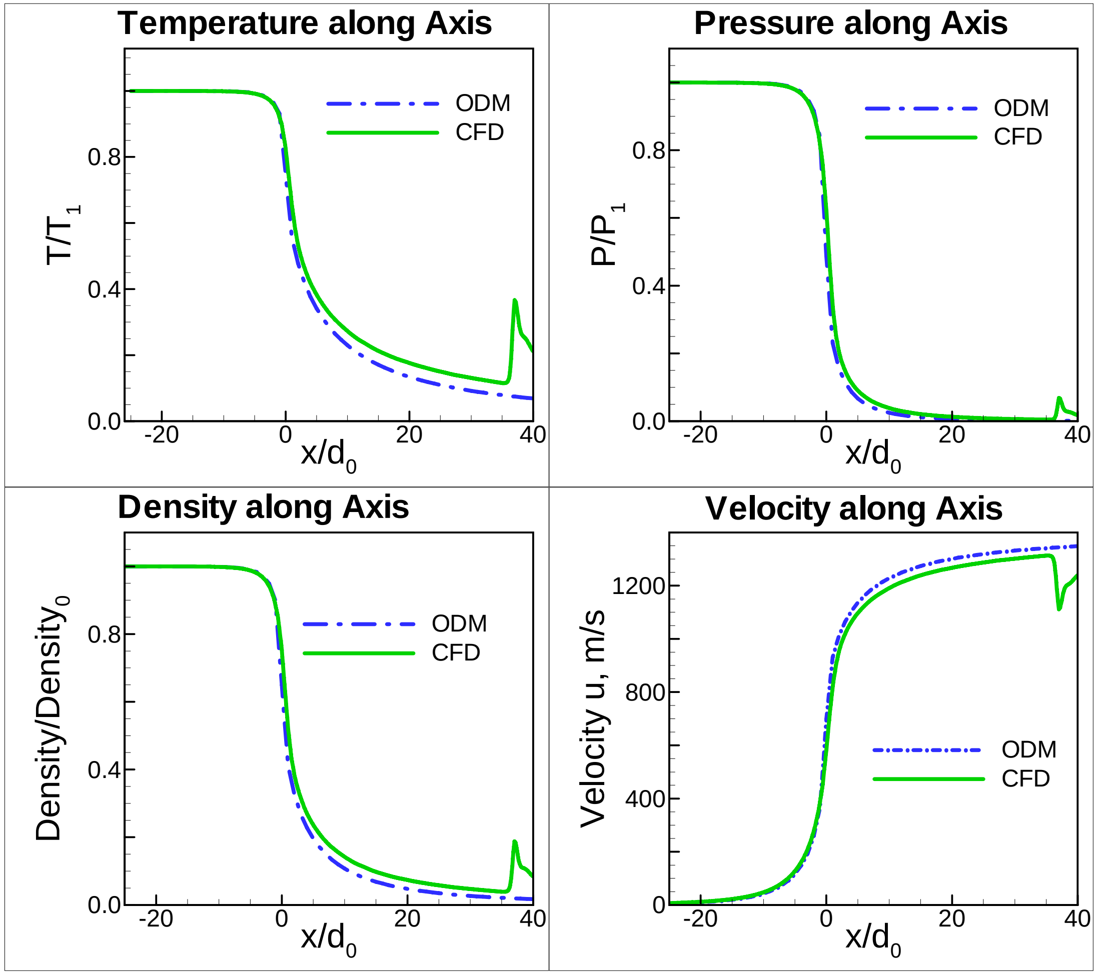
Brooks et al., The Physical Chemistry of Carbothermic Route to Mg, 2006

CFD Modelling of Supersonic Quenching

- Commercial ANYSY/CFX5.7.1 Code
- Hexahedral mesh
- Solving steady state conservation equations for mass, momentum and thermal energy
- Which turbulence model ?
- Validation against 1-D model (ODM) and literature data
- Coupling with condensation kinetics

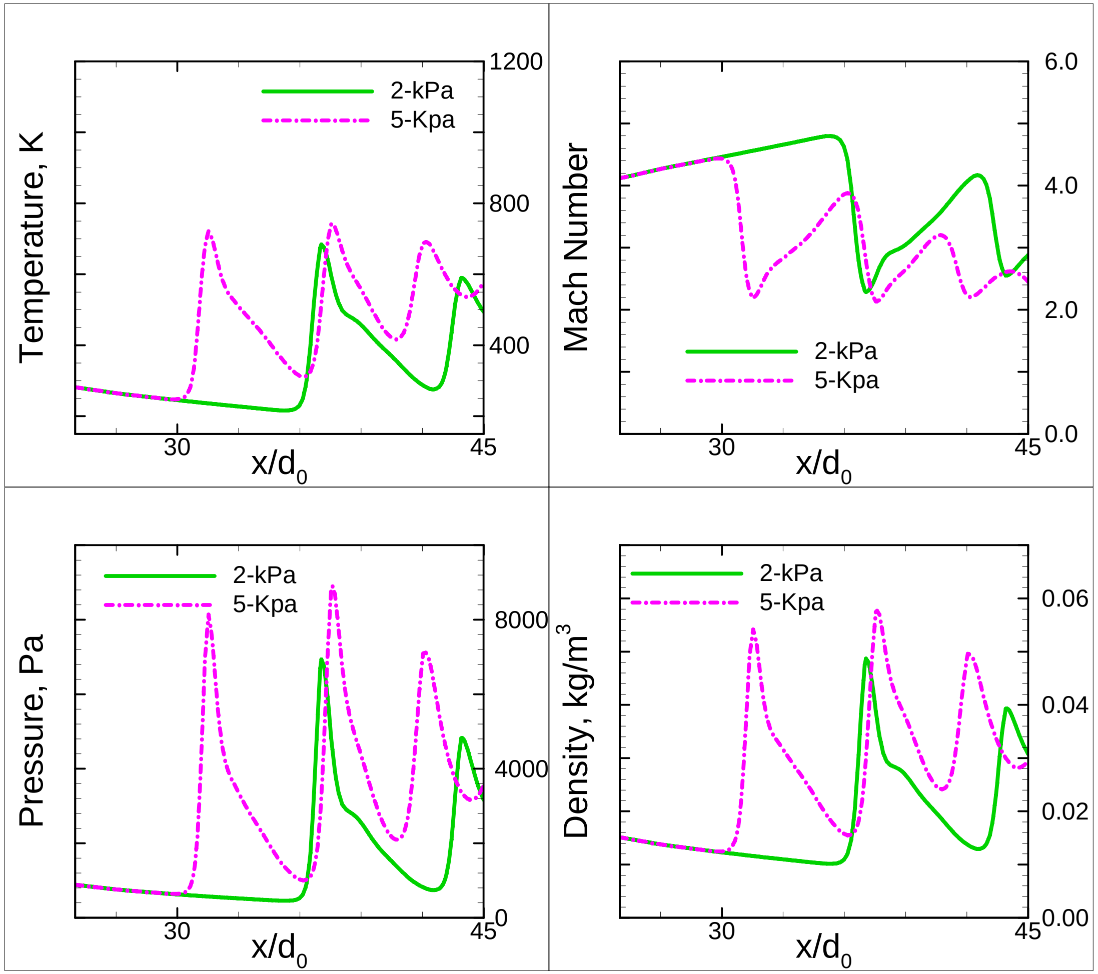
Khan et al. Design of Supersonic Nozzles for Ultra-Rapid Quenching of Metallic Vapours, 2006
Brooks et al., CFD Modelling of heat transfer in supersonic nozzles for mg production, 2007

Centreline Predictions



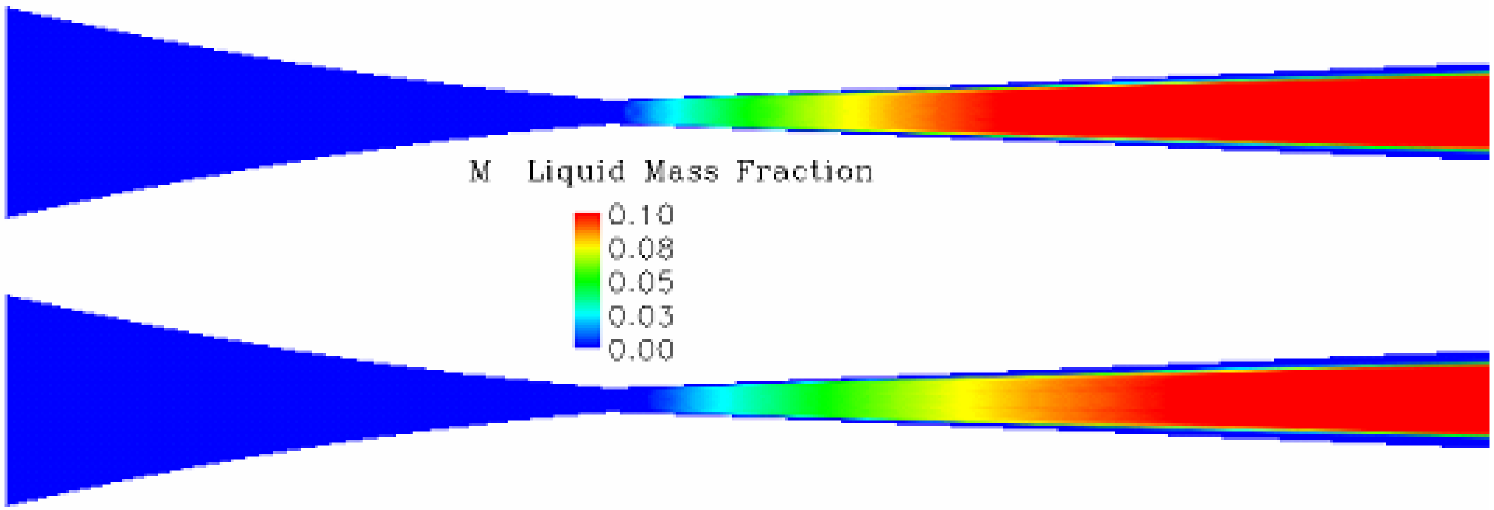
Argon Gas, Inlet 1 atm and 1600 C, 5mm throat
Khan et al., 2006

Shock Waves in Nozzle



Argon Gas, Inlet 1 atm and 1600 C, 5mm throat
Khan et al., 2006

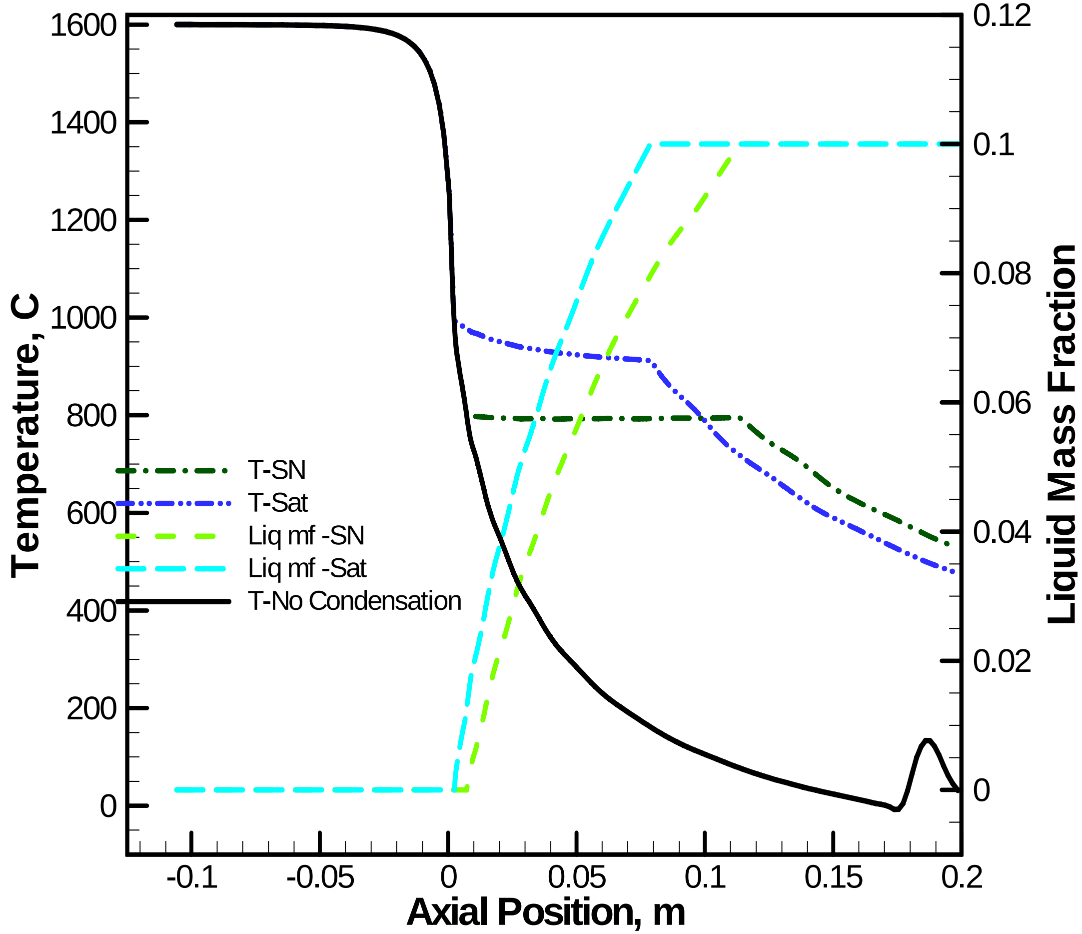
Condensation Kinetics



Mass Fraction of Metal Condensing in Nozzle with Standard Sat. Curve (Top) & Scaled Nucleation Theory (Bottom).

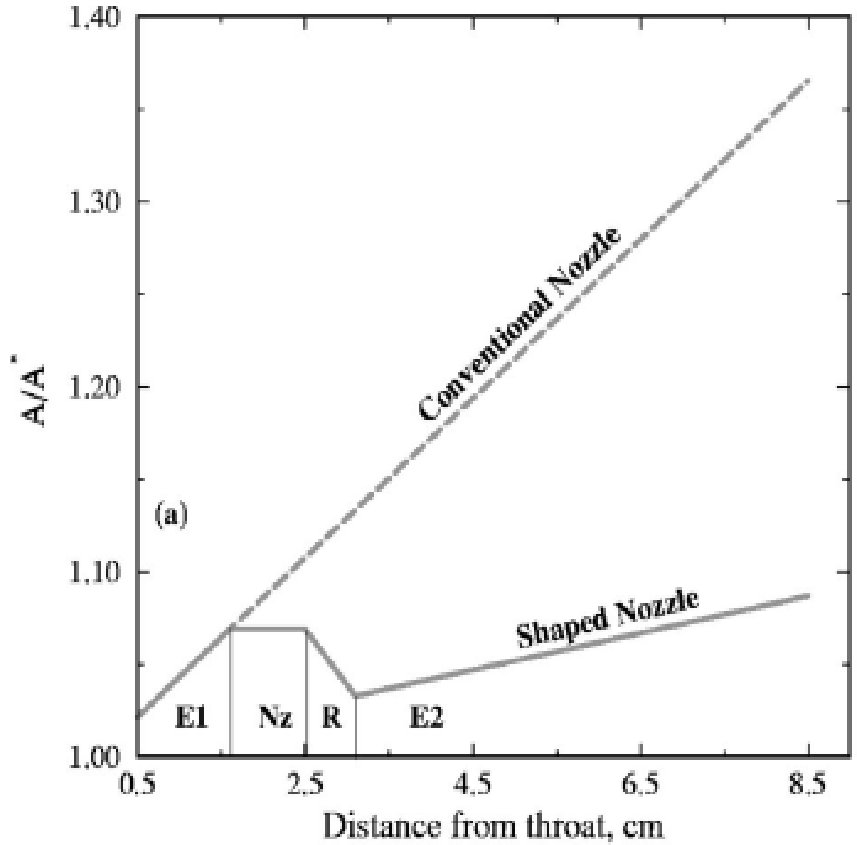
Argon Gas, Inlet 1 atm,1600 C, 10% Mg + CO/Ar, 5mm throat, 10% Mg
Khan et al., 2006

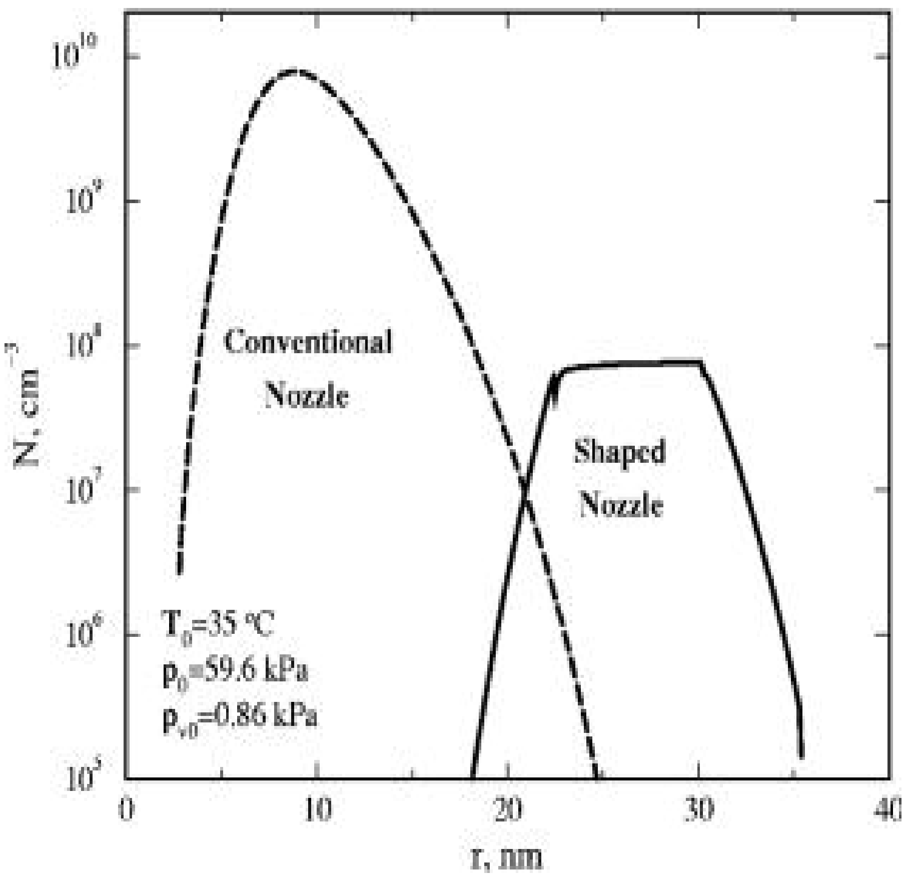
Condensation Kinetics



Argon Gas, Inlet 1 atm,1600 C, 10% Mg + CO/Ar, 5mm throat, 10% Mg
Khan et al., 2006

Shaped Nozzles





Streletzky et al., 2002

Future Work

- Development of thermodynamic models to develop new process routes to high purity Mg
- Coupling of Molecular Dynamics with CFD for supersonic condensation
- Shaped nozzles to control condensate size ??

Generic Challenge – Coupling of chemistry and fluid dynamics

My co-workers and supporters

Mike Nagle, Peter Witt, Annette Koo, Tim Barton and M. Khan

CSIRO Minerals and Swinburne University of Technology