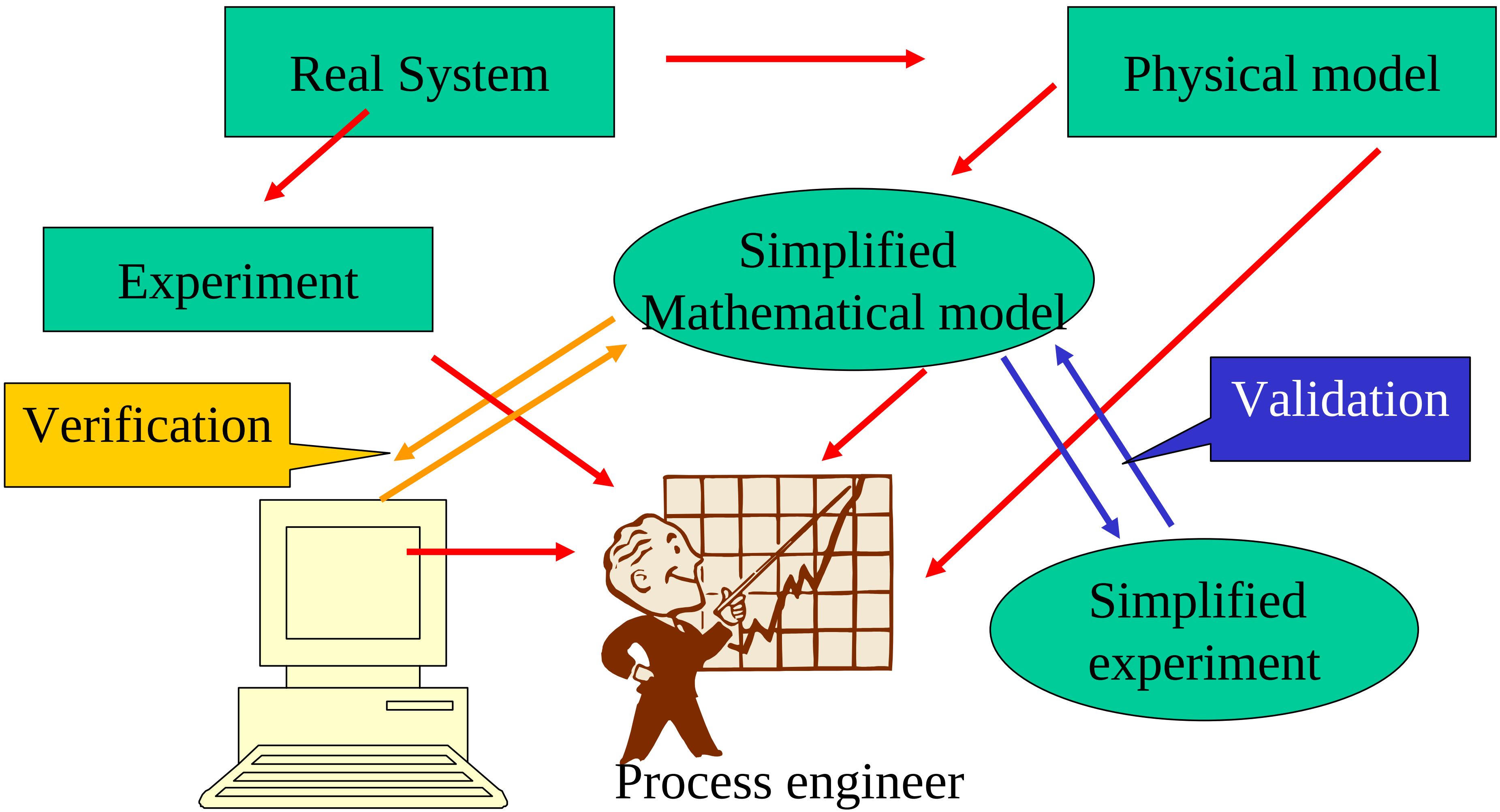
METRO
MEtallurgical TRaining On-line

Laboratory benchmarks for validating numerical simulation of casting problems

Tomasz A. Kowalewski
IPPT PAN

Education and Culture

Analysis of casting system



Why we need experimental validation?

Numerical simulation simplifications due to:

- Limits of discretization accuracy
- Equations (Navier-Stokes) non-linearity
- Strongly non-linear moving boundary problem
- Variable physical properties of fluid/solid phases
- Complex thermal boundary conditions
- Mushy regions, chimneys, solutal convection
- Wide disparity of physical scales
- Sensitivity to boundary/initial conditions

Numerical code certification

- **Numerical model verification**
- **Numerical model validation**

↓

- Physical model verification
- Numerical model verification
- Experimental validation

Physical model verification

Define physical model of the simulated phenomena

- Verify importance of the details
- Extract crucial parameters
- Similarity analysis
- Construct physical model adequate to the simulated industrial configuration
- Identify possible sources of discrepancies

Numerical model verification

Are we properly solving equations?

- Verification of model mathematics
- Verification of discretization (grid convergence test)
- Inter-code comparison
- Numerical benchmark comparison

Numerical method
Basic set of equations

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \tilde{U}) = 0$$

Momentum equation:

$$\frac{\partial \rho \tilde{U}}{\partial t} + \nabla \cdot \rho \tilde{U} \otimes \tilde{U} = -\nabla p + \nabla \cdot \left(\mu \nabla \tilde{U} + \mu \left(\nabla \tilde{U} \right)^T \right) + \tilde{B}$$

$$\tilde{B} = \rho_0 \left[-\beta_T (T - T_0) + \beta_C (C - C_0) \right] \tilde{g}$$

Energy equation:

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \tilde{U} h) - \nabla \cdot (\lambda \nabla T) = 0$$

Concentration equation:

$$\frac{\partial \rho C}{\partial t} + \nabla \cdot (\rho \tilde{U} C) = \nabla \cdot (\rho D \nabla C)$$

Numerical method selection 1

1. Interface tracking method - academic
2. Fixed grid method (most commercial codes)

Both methods solve the same problem:

- Navier-Stokes Equations for mass transport
- Energy equation for heat transport, including phase change latent heat

Interface tracking method in addition resolves dynamics of the solid-liquid interface

Numerical method selection 2

1. Finite Difference – mostly academic
2. Finite Volume – more flexible geometry
3. Finite Element – most commercial codes
4. Other: Boundary Element, Mesh-Free

All methods solve the same problem:

- Navier-Stokes Equations for mass transport
- Energy equation for heat transport, including phase change latent heat

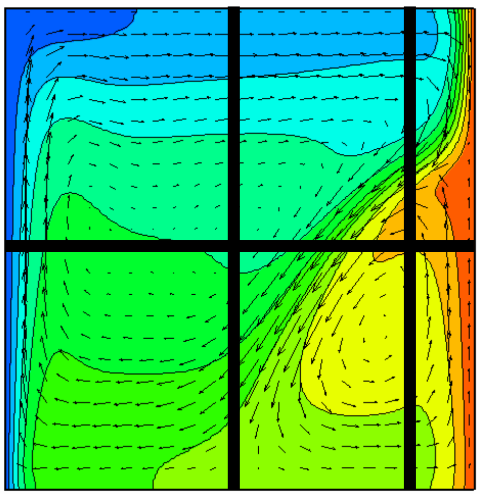
Verification of numerical model

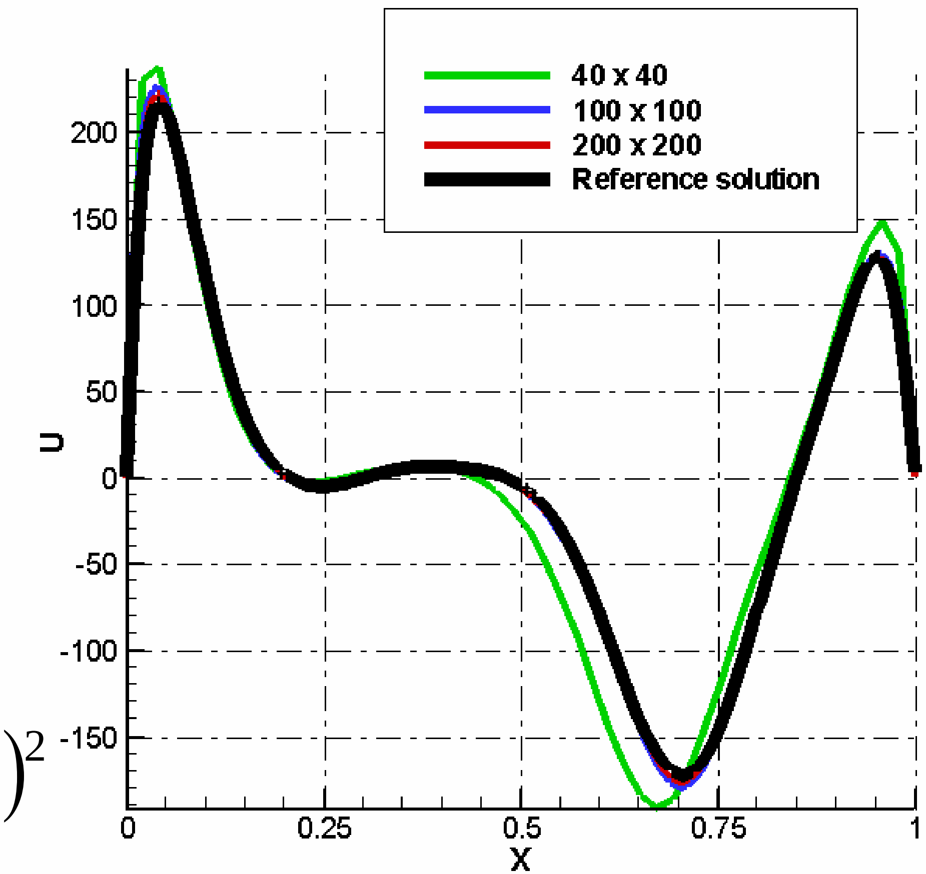
1. Grid convergence test – discretization errors
2. Conceptual errors – like non-ordered approximations
3. Computer round-off errors
4. Programming errors

Compare with known solutions
– numerical benchmarks

Numerical benchmark

CALCULATE: SOLUTION & SOLUTION UNCERTAINTY



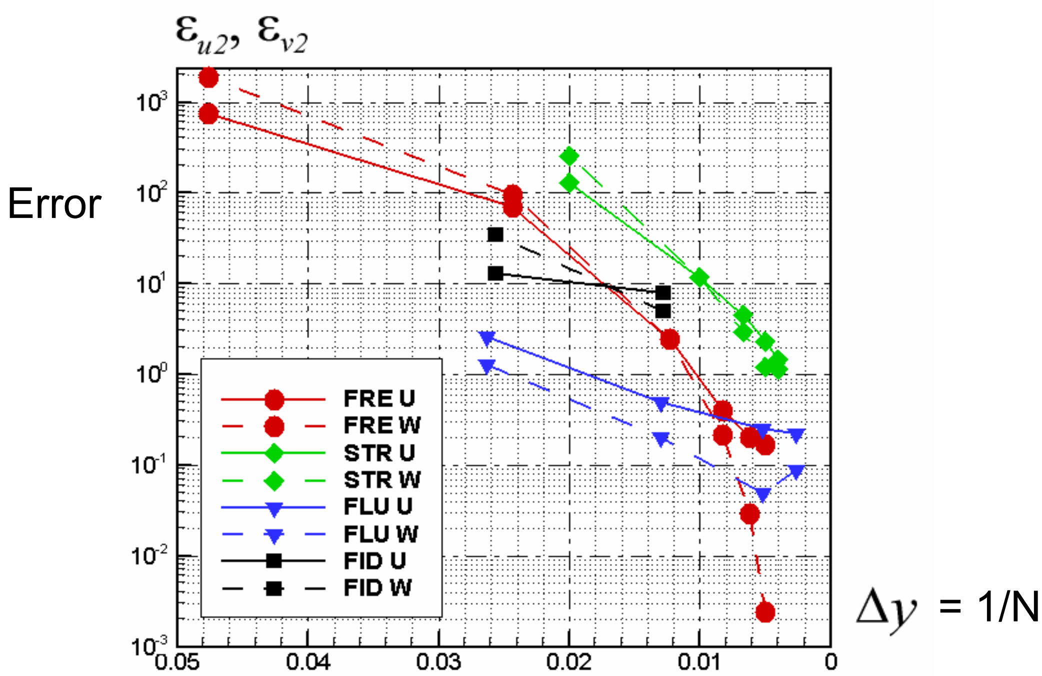


Error indicator
for code comparisons

$$\varepsilon(f)=\frac{1}{N}\sum_{i=1}^{N}\left(f(x_i)-w(x_i)\right)^2$$

Numerical benchmark

GRID TEST FOR DIFFERENT SOLVERS



$$\varepsilon(f) = \frac{1}{N}\sum_{i=1}^{N}\left(f(x_i) - w(x_i)\right)^2$$

Numerical model validation

Are we solving proper equations?

- Verification of physical model used
- Verification of boundary/initial conditions
- Verification of material properties
- Definition of reliable experimental test
- Validation (comparison) with experimental data

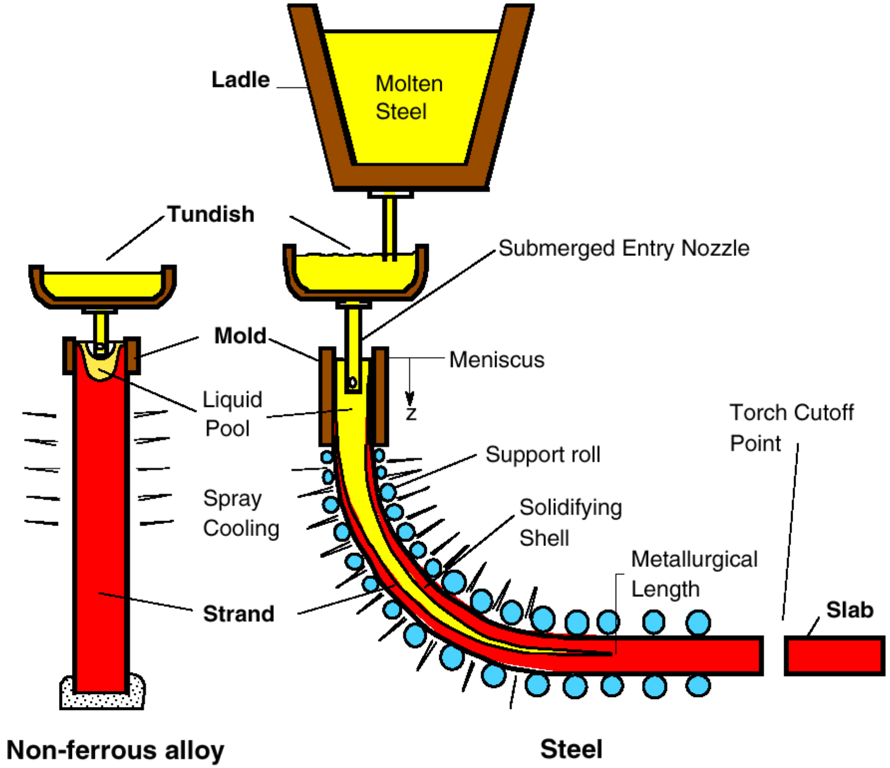
Selection of the test problem

Possible choice:

- Industrial full scale configuration
  - Complex geometry, inaccurate boundary / initial conditions & material properties, difficult experimental methodology
- Industrial laboratory model
  - Well controllable environment, inaccurate properties, difficult experimental methodology
- Analogue laboratory model
  - Full experimental control

Industrial configuration

Industrial configurations are very difficult to investigate experimentally



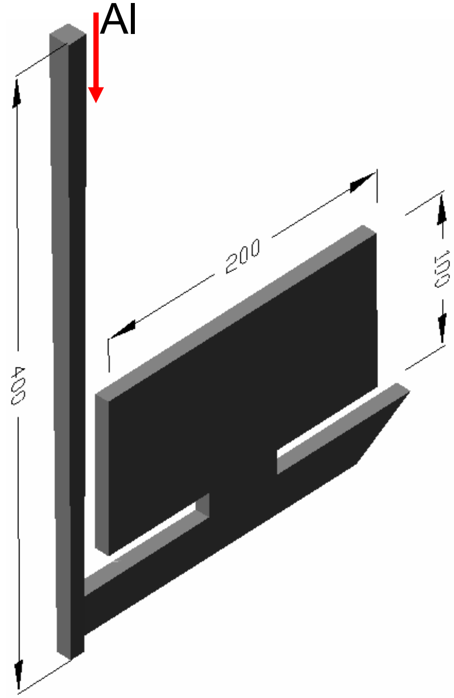
B. Saler, AMAS 2003

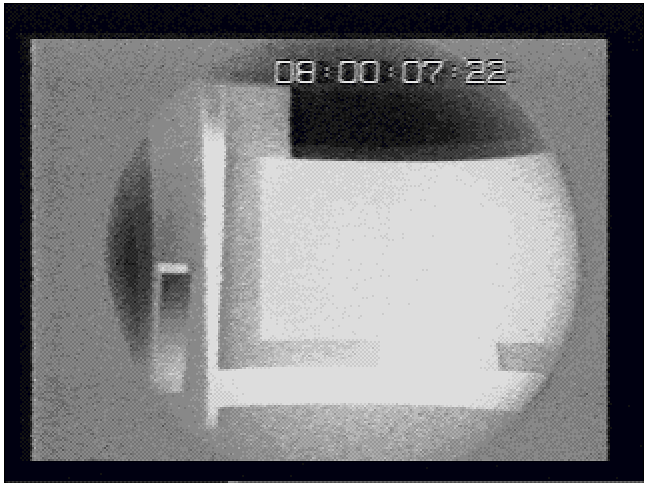
Industrial configuration

Limitations - measurements of:

- interface topology ► difficult for non-transparent materials
- velocity field ► very limited for non-transparent materials
- temperature ► surface only for non-transparent materials
- concentration ► difficult in general
- thermal BC ► usually possible for external walls only
- initial conditions ► special arrangement necessary

Industrial laboratory model



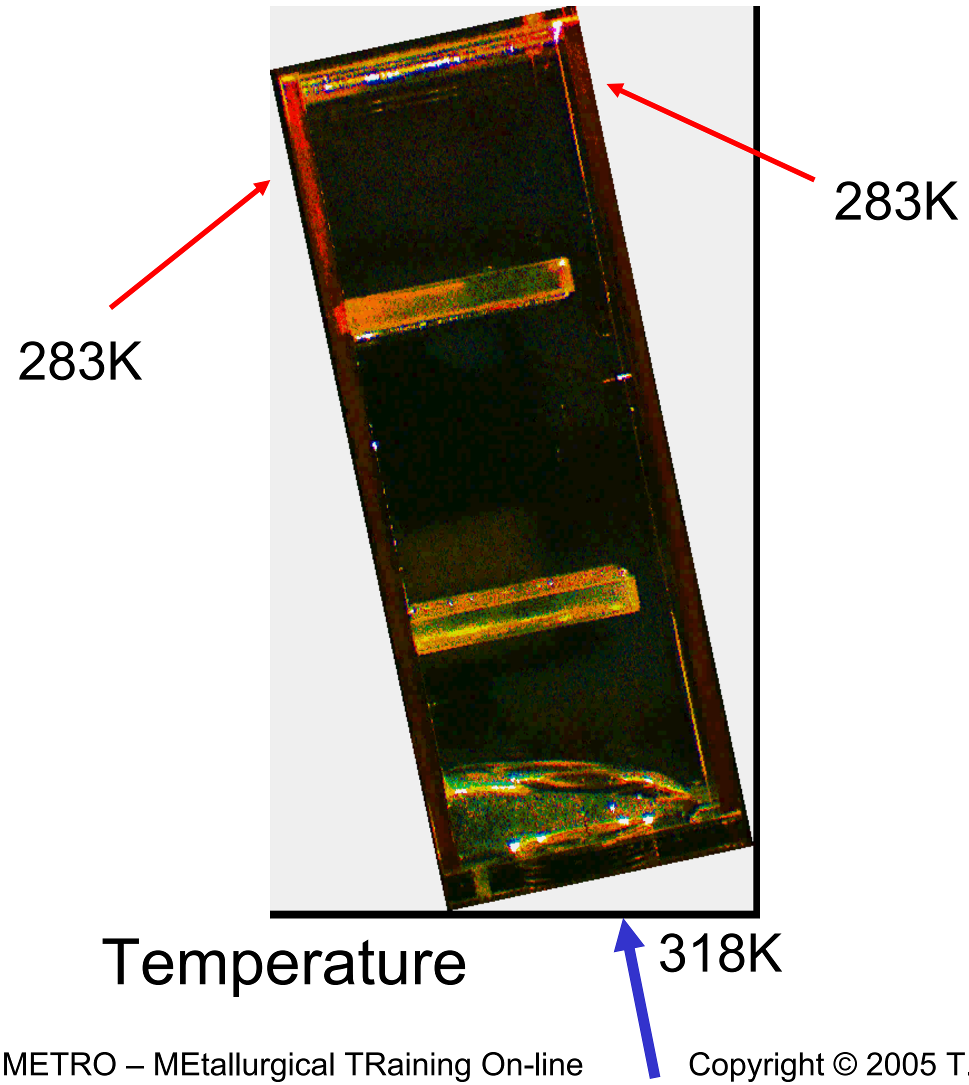


X-ray movie

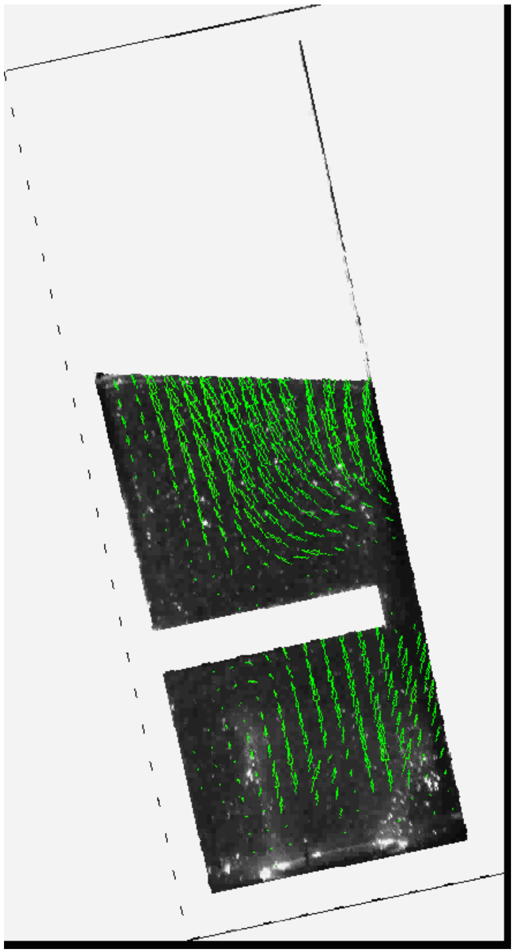
Mould filling benchmark test proposed at 7th conference on modelling casting and welding processes (Sirrell et al. 1995).

Despite of expensive and complicated experimental procedure -> delivered data appeared not sufficient for validating submitted numerical solutions

Analogue laboratory model



Temperature



Velocity

Analogue laboratory model

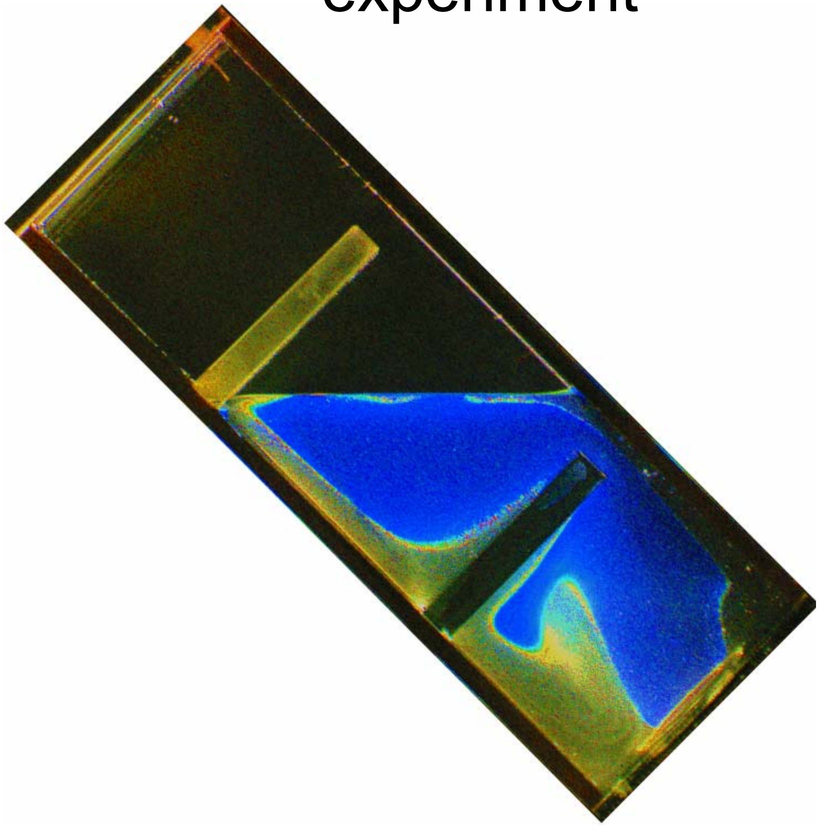
OPTICAL METHODS
- PIT — **colours** → **temperatures**
- PIV — **vectors** → **velocities**

Advantages – full field flow, temperature and concentration data collection, well known material properties, fully controllable experimental conditions

Limitations – transparent analogue materials, simple cavity shapes, radiation neglected, Prandtl number > 1, ….

Analogue laboratory model
Mould filling phase

experiment



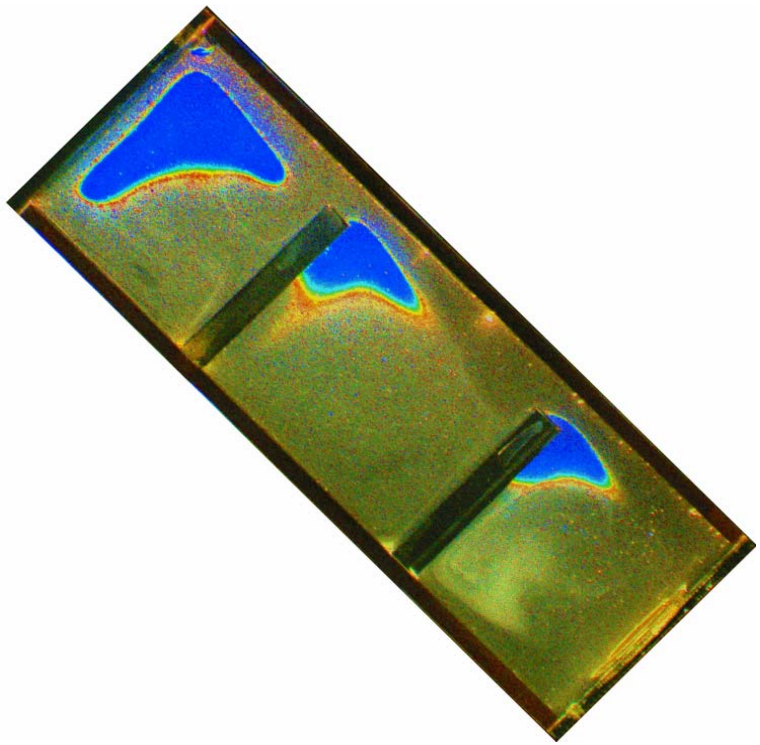
numerical simulation

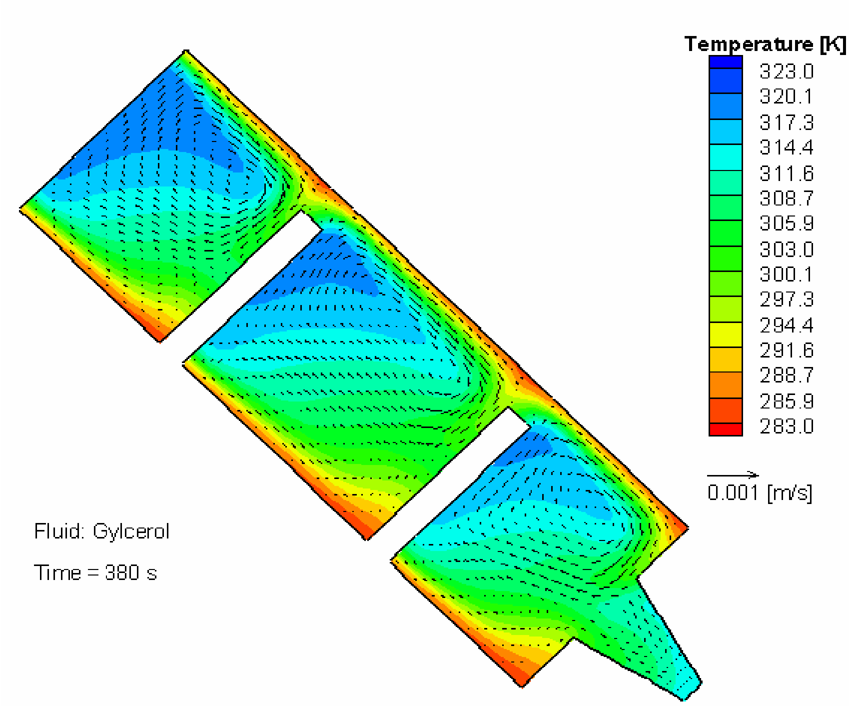
Full field transient data can be quantitatively compared

Analogue laboratory model
Mould cooling phase

experiment

numerical simulation

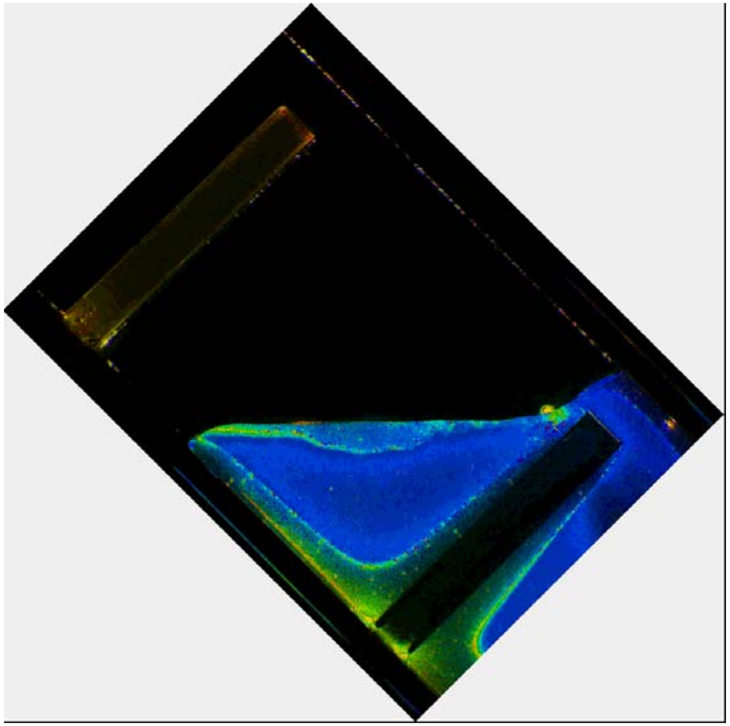




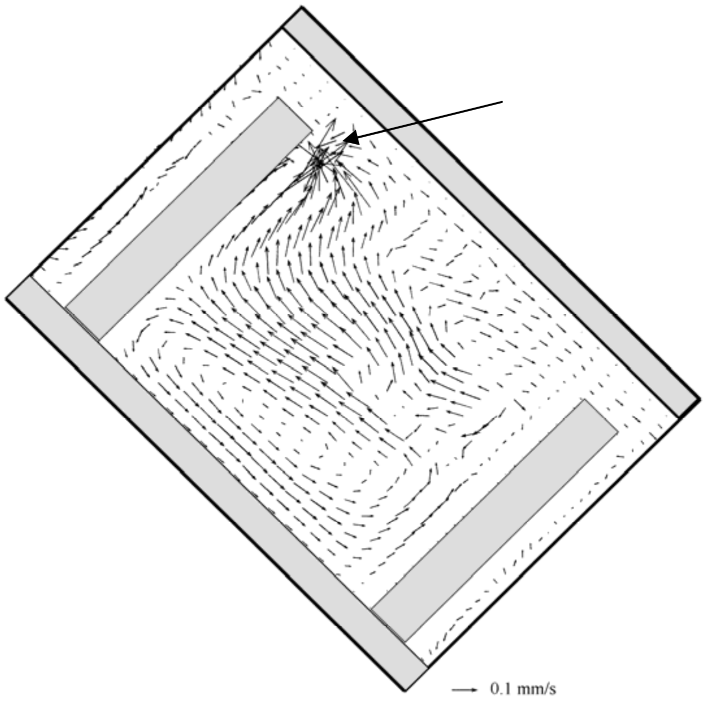
Full field transient data can be quantitatively compared

Analogue laboratory model „Hot spots" identification

Experiment - temperature



Experiment - velocity



Full field transient data can be used to detect local features

Experimental benchmark using analogue fluid

Numerical model can be validated using laboratory data

Optical methods make possible

- ✓ **3D measurements of velocity, temperature and concentration**
- ✓ **Validation of fluid mechanics, thermodynamics, phase change and micro- structure**

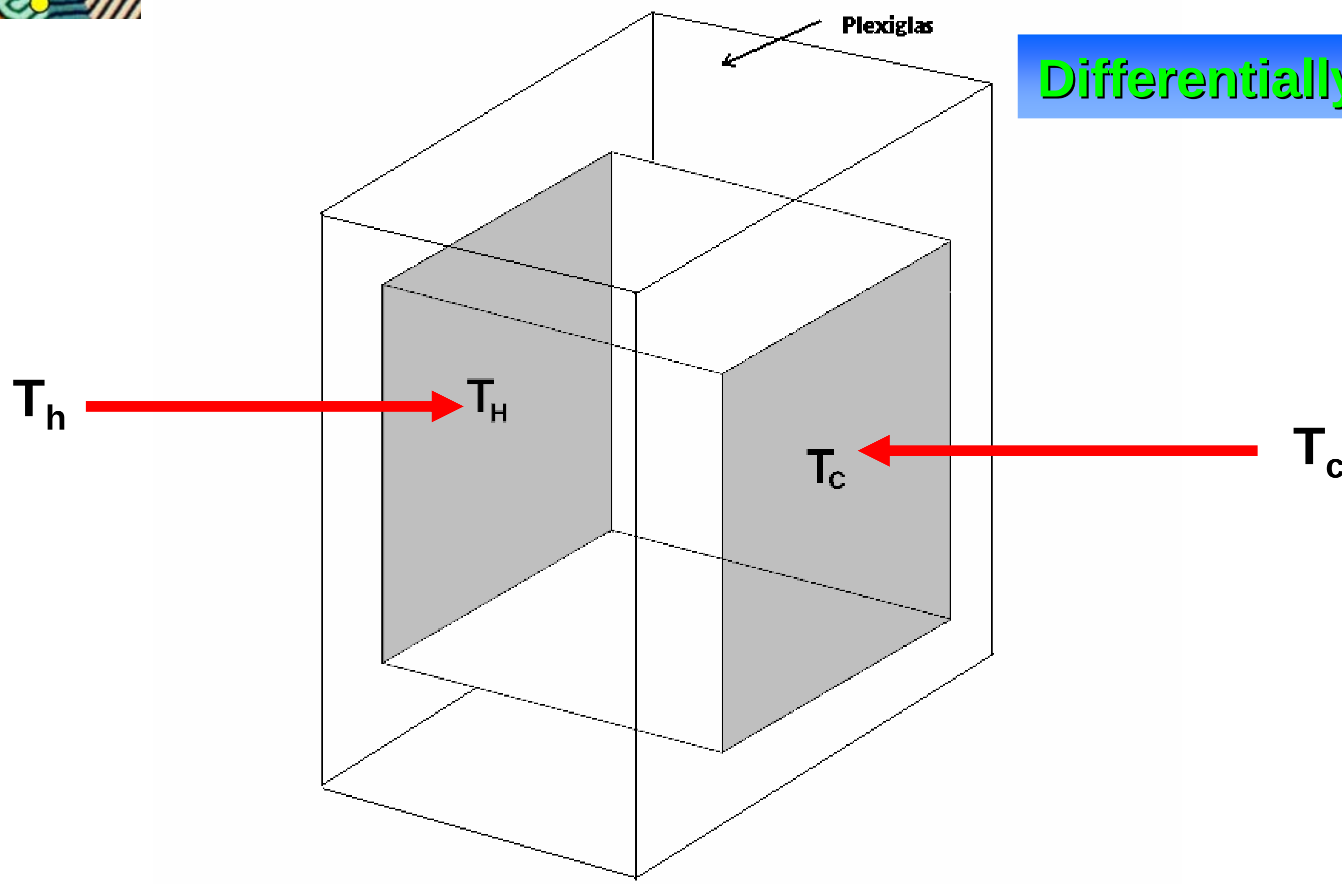
Full field velocity, temperature, concentration data together with shape, interface dynamics

Experimental benchmark
Typical analogue fluids

	Water	SCN	PEG 900	Hexadecane
density, ρ [(kg m^{-3}]	999	985	1100	792
Specific heat, c [J kg^{-1} K^{-1}]	4217,8	2000	2260	2236
thermal cond., k [W $m^{-1}K^{-1}$)]	0.552	0.223	0.188	0.18
thermal expansion, β [K^{-1}]	$-0.07 \cdot 10^{-3}$	$0.81 \cdot 10^{-3}$	$0.76 \cdot 10^{-3}$	$0.9 \cdot 10^{-3}$
melting temperature, [°C]	0	55	34	18
kinematic viscosity, ν [m^2 s^{-1}]	$1.8 \cdot 10^{-6}$	$2.6 \cdot 10^{-6}$	$9.0 \cdot 10^{-6}$	$3 \cdot 10^{-6}$
Prandtl number, Pr	13	23	1188	45

Example benchmark

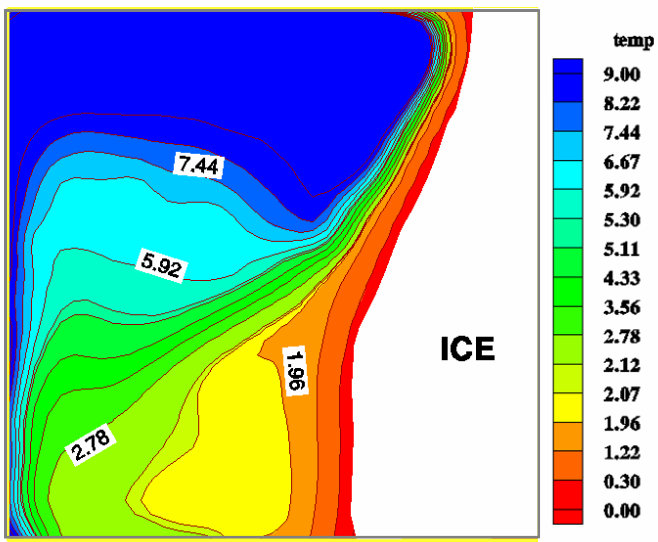
Differentially Heated Cavity

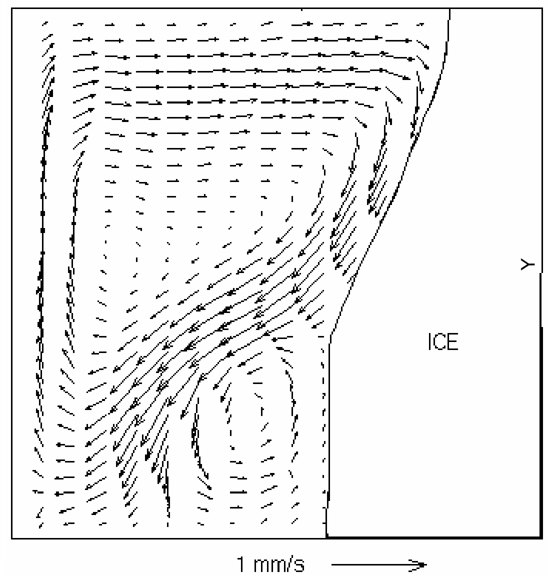


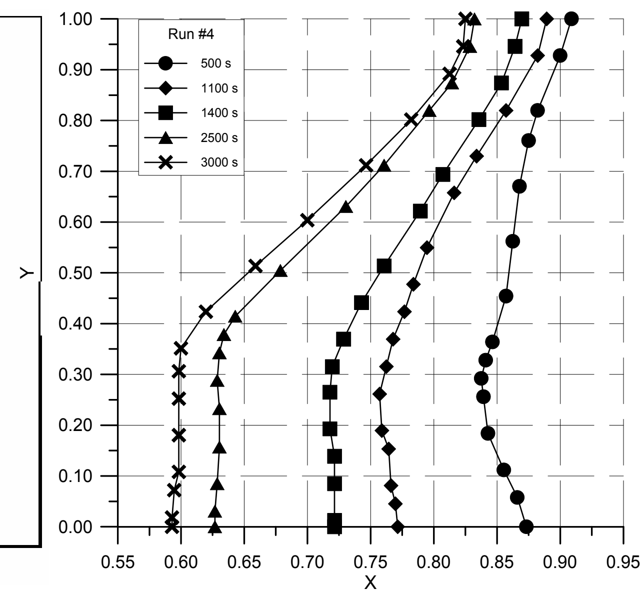
Freezing of water. Velocity, temperature and ice front observed in centre plane of the differentially heated cavity. $T_h=10^oC$, $T_c=-10^oC$

Example benchmark

Differentially Heated Cavity



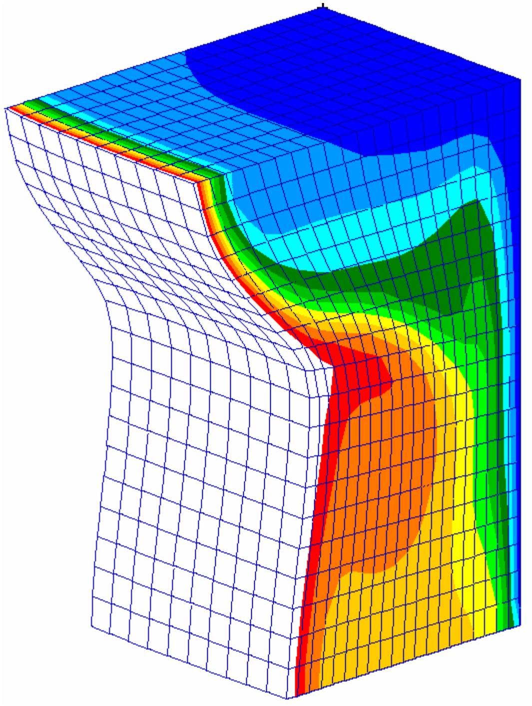


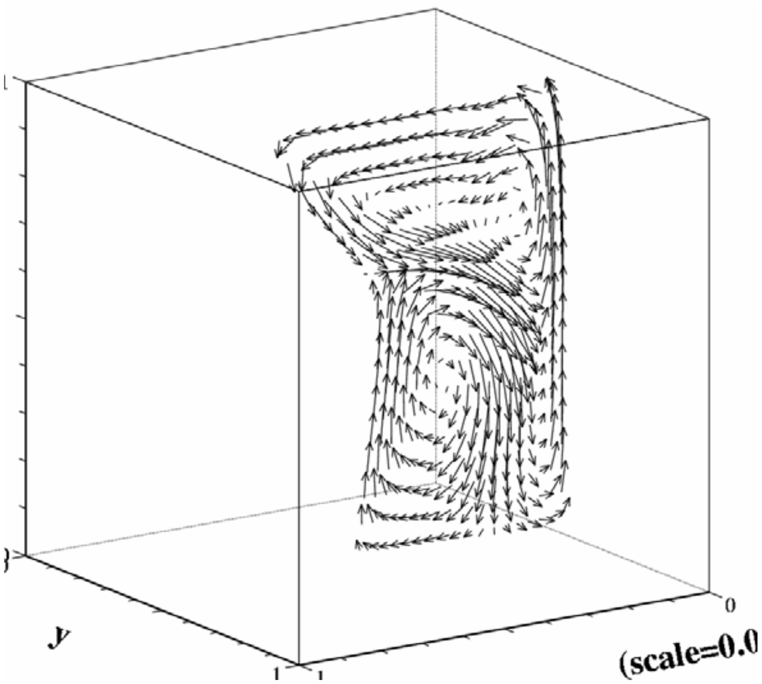


Temperature, velocity fields, and interface geometry (t) from experiment

Example benchmark

Differentially Heated Cavity

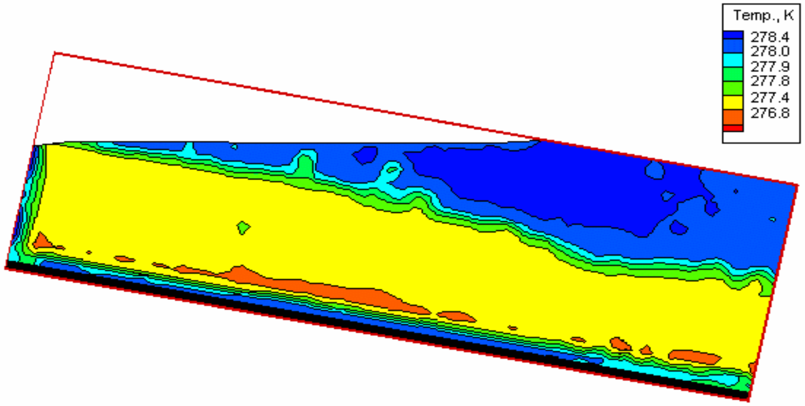


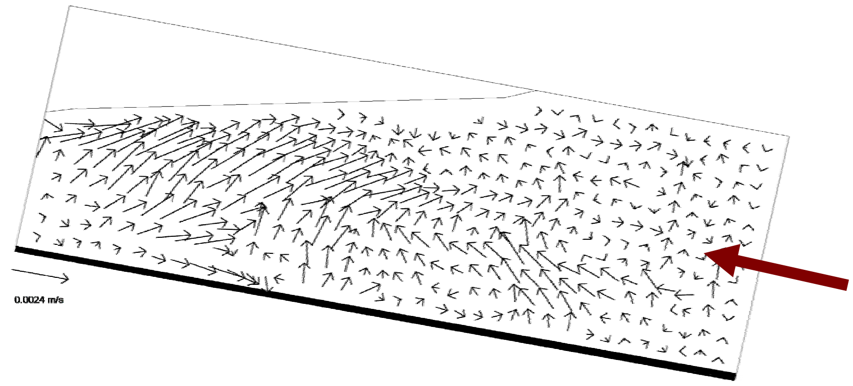


Temperature, velocity fields, and interface geometry (t) from simulation

Example benchmark

Mould filling with freezing water

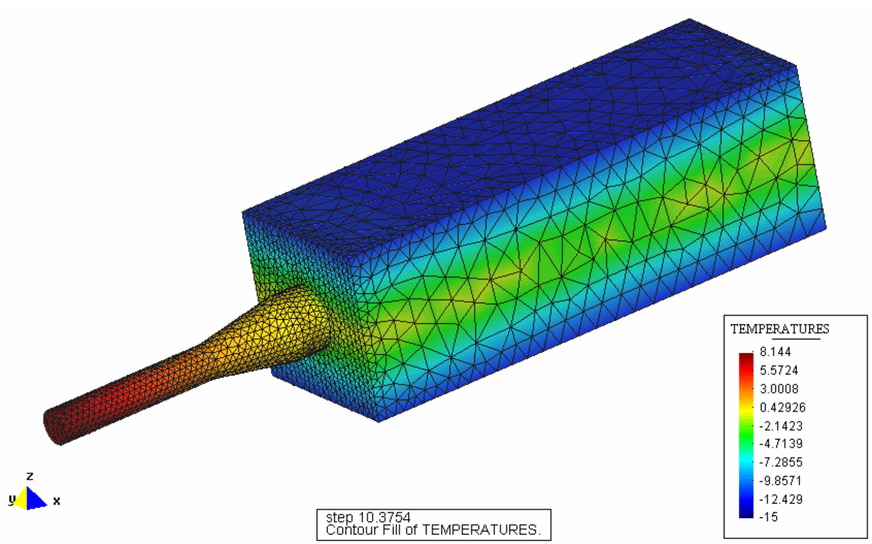




Temperature, velocity fields, and interface geometry (t) from experiment

Example benchmark

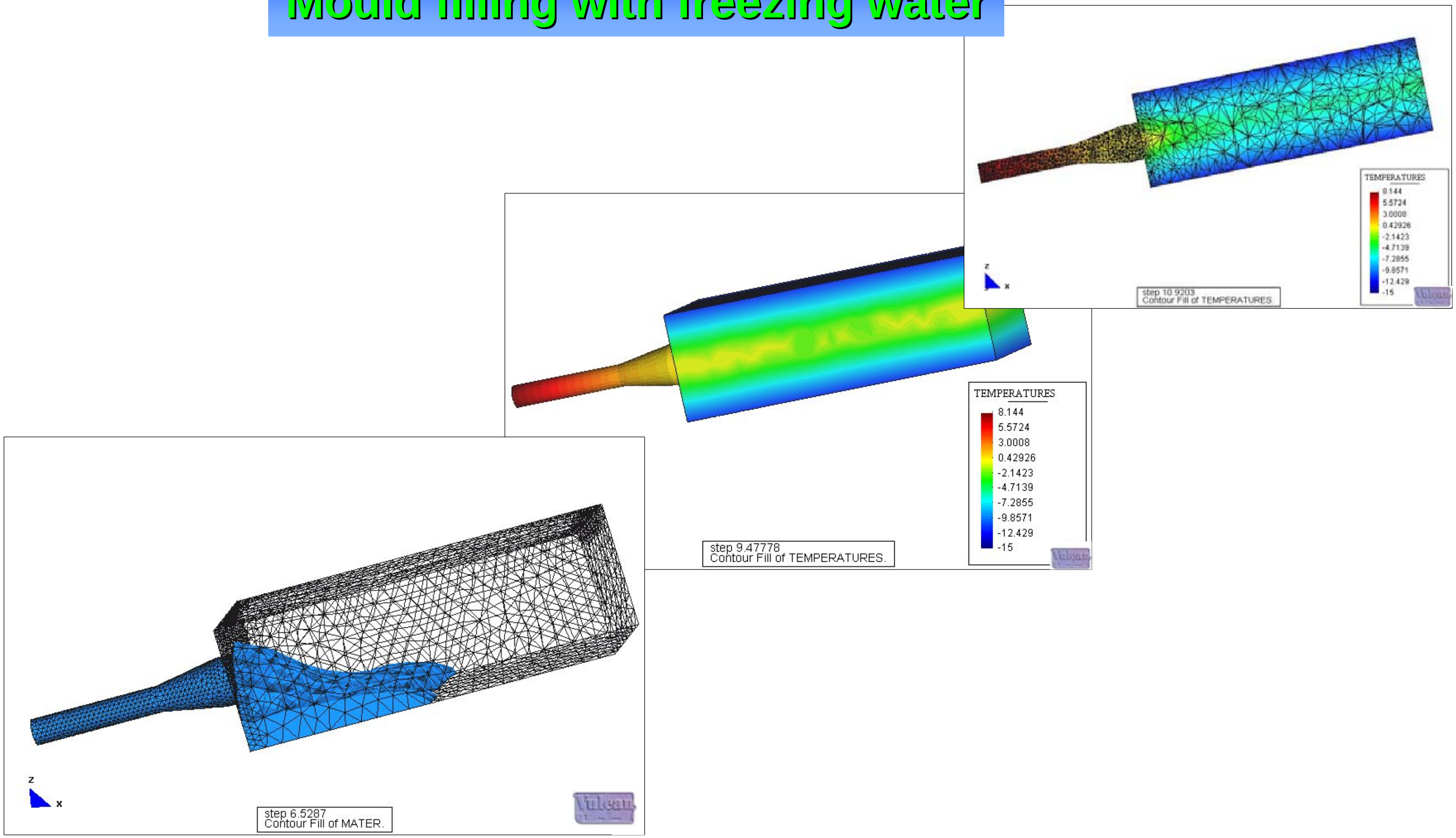
Mould filling with freezing water



Testing casting code 1

Example benchmark

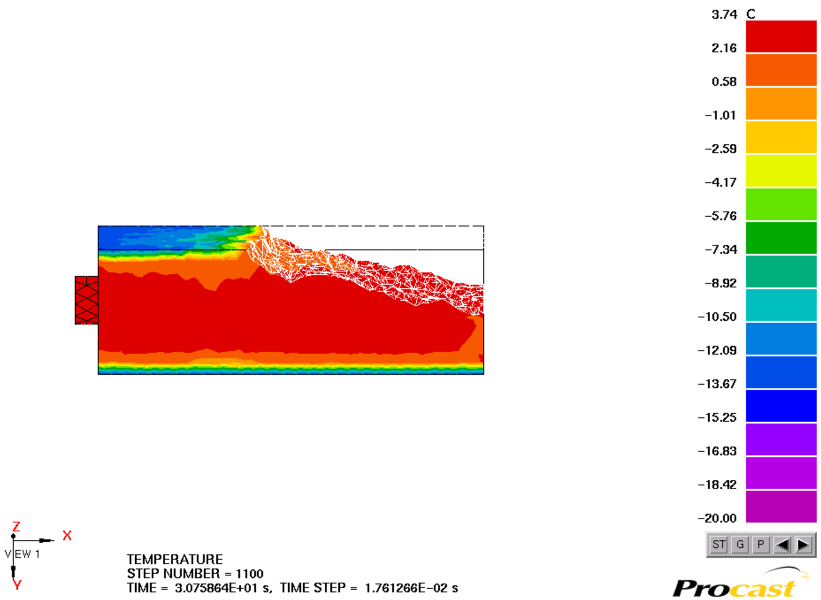
Mould filling with freezing water

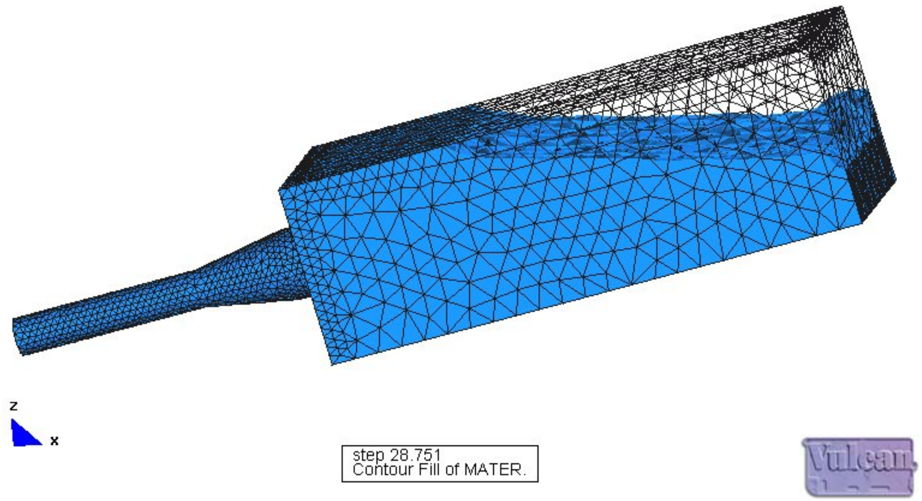


Example benchmark

Mould filling with freezing water

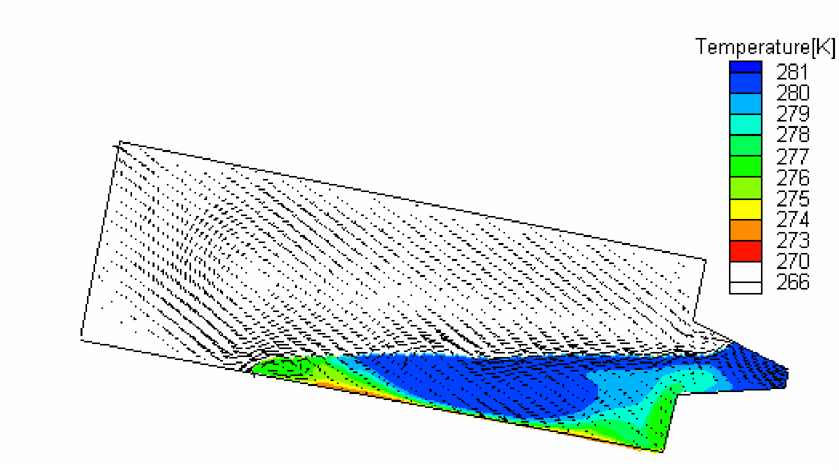
Casting Code 1 vs. casting Code 2

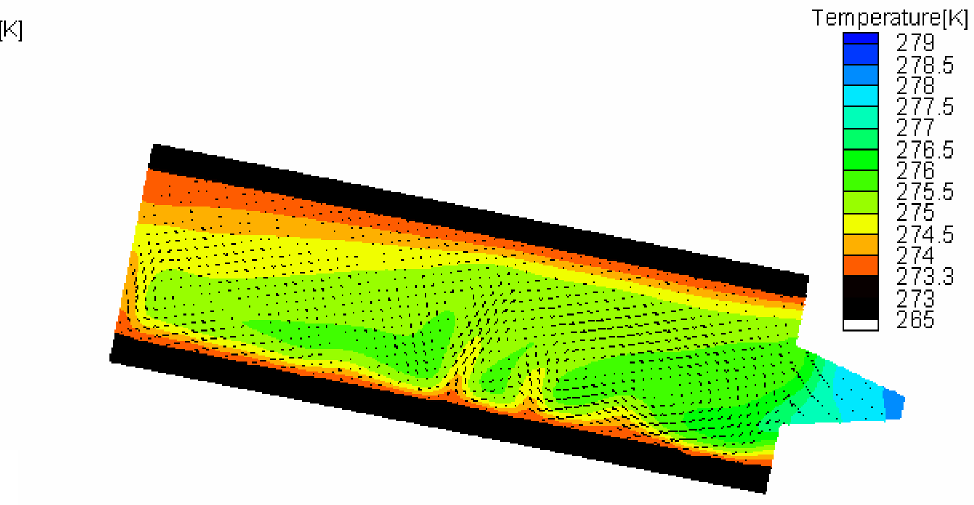




Example benchmark

Mould filling with freezing water

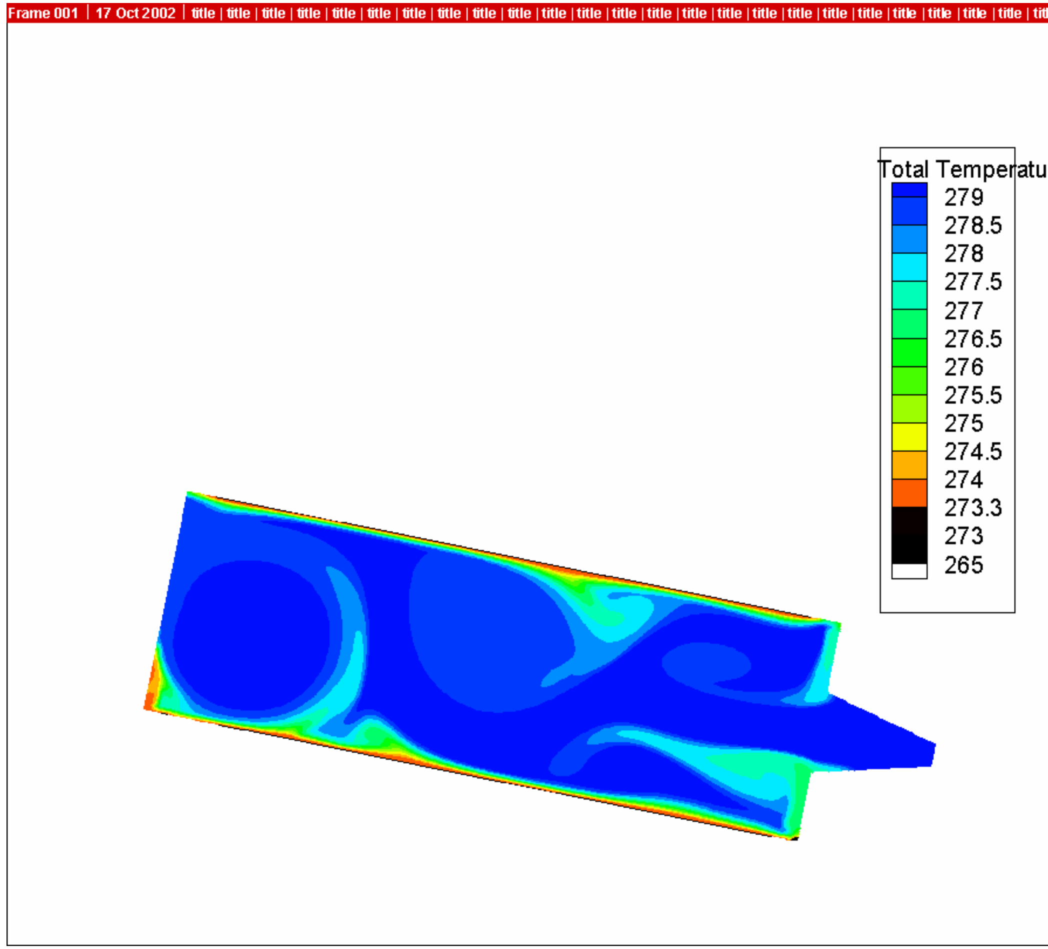




Fluent 6.0

Example benchmark

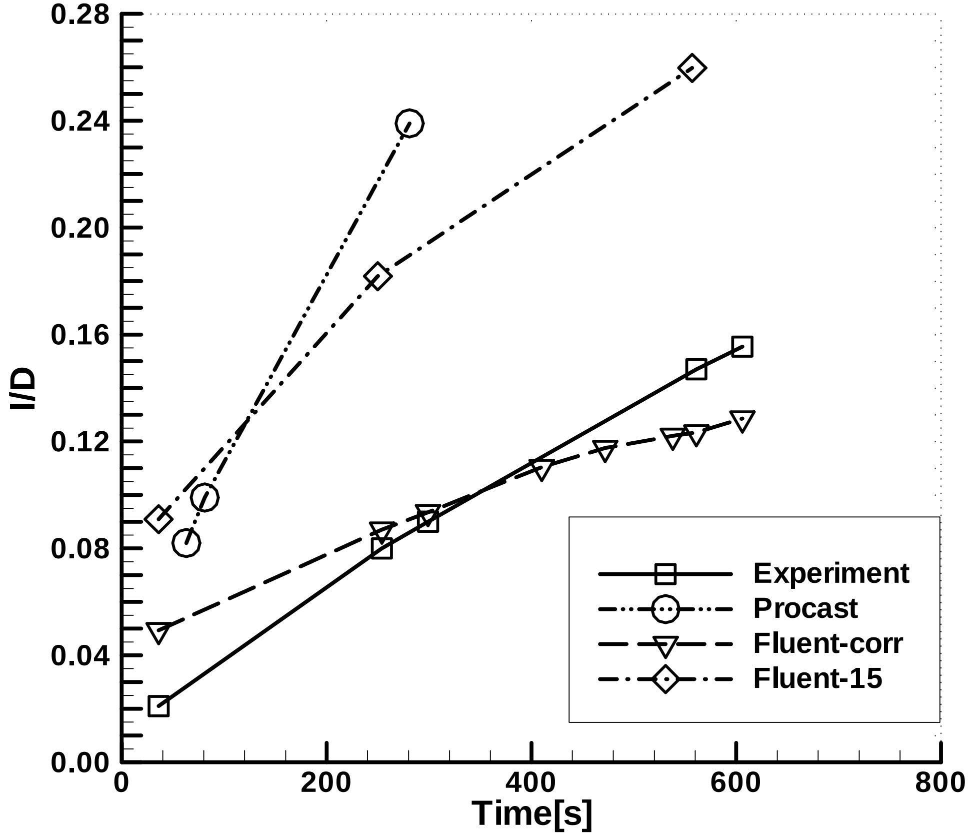
Mould filling with freezing water



Fluent 6.0

Example benchmark

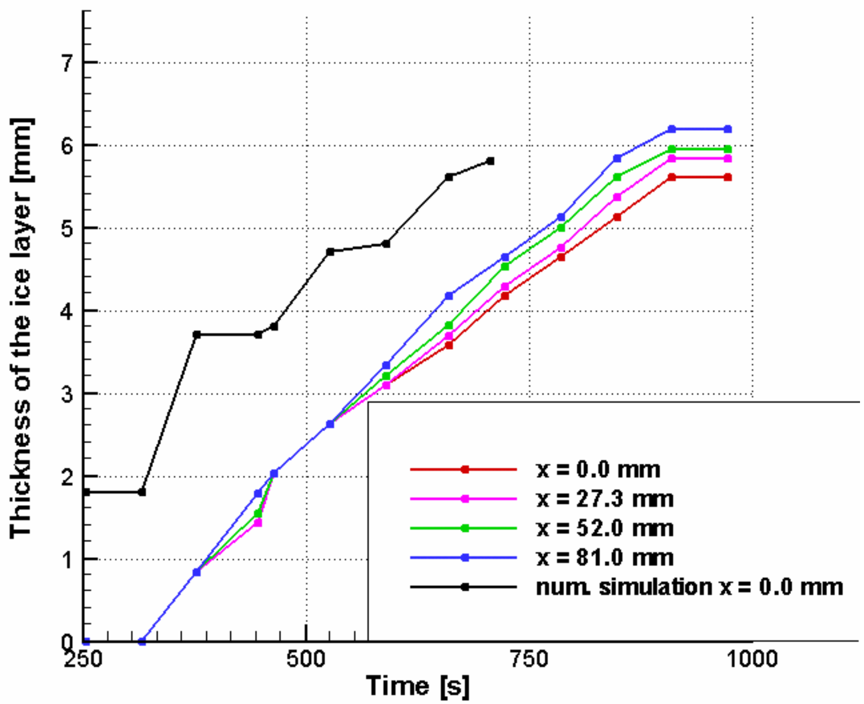
Mould filling with freezing water

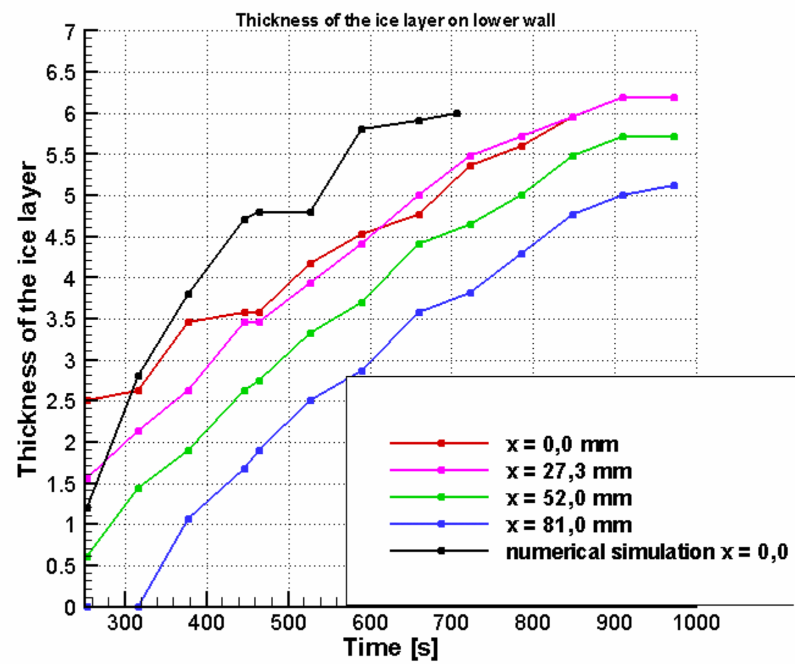


Interface position predicted and measured

Example benchmark

Mould filling with freezing water





Water freezing after filling: ice front measured and compared with numerical prediction Fluent).

Validation Methodology

- Select experimental configuration
- Define characteristic parameters of the problem
- Estimate experimental error for each parameter
- Estimate sensitivity of the problem to these errors
- Perform validation procedure using knowledge gain from the experiment (data, accuracy) and from numerical simulations (sensitivity)

Validation Methodology

- Validation error *E* is defined as difference between the experimental Data *D* and the value produced by the simulation *S*

$$|E| = D - S$$

- Validation uncertainty, sum of Data, Simulation, and Material uncertainties

$$U_V = \left(U_D^2 + U_{SN}^2 + U_{SPD}^2\right)^{0.5}$$

- Validation Error *E* has to be smaller than uncertainty *U*

$$|E| \le U_V = \left(U_D^2 + U_{SN}^2 + U_{SPD}^2\right)^{0.5}$$

Summary

- To understanding differences between numerical and experimental data

  ⇒ necessary to compare full field data

- Detailed experimental data for analogue fluids, select critical set

  ⇒ available quantitative, full-field information about the temperature and velocity fields

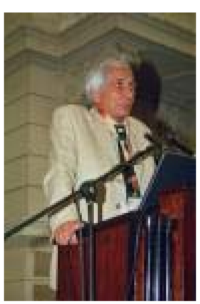
  ⇒ estimate necessary accuracy to use the data for the validation

- Perform sensitivity test and validation
- Validation using analogue fluids

  ⇒ necessary condition but not sufficient

Literature

- T.A. Kowalewski, *Particle Image Velocimetry and Thermometry in two phase problems*, Annals of New York Academy of Sciences, vol.972, pp.213-222, edts. S. Siedeman & A Landesberg, NY 2002.
- T.A. Kowalewski, *Experimental Methods for Quantitative Analysis of Thermally Driven Flows in Phase Change with Convection*, eds. T. Kowalewski, D. Gobin, CISM Lecture Notes, vol. 449, Springer 2004
- T. Michalek, T. Kowalewski, B. Saler, *Natural Convection for Anomalous Density Variation of Water - Numerical Benchmark*, Progress in Computational Fluid Dynamics, 5, pp. 158-170, 2005



for more please visit: http://www.ippt.gov.pl/~tkowale/

Acknowledgments

The author has been fortunate to share part of this work with his colleagues and students from the Max-Planck-Institut, New South Wales University, La Sapienza, and at his home institution.
In particular I would like to acknowledge the contribution of

W. Hiller
St. Koch
G. de Vahl Davis
E. Leonardi
F. Stella
M. Gangi
A. Cybulski
M. Rebow
T. Michalek
M. Kowalczyk

to what has been a team effort over a number of years.