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VALIDATION OF NUMERICAL SIMULATION OF FREEZING POINT OF ZINC

D.M. Camarano [1], *R.M. Andrade* [2]

[1] National Commission of Nuclear Energy, Nuclear Technology Development Center, Belo Horizonte, MG, Brazil, dmc@cdtn.br
[2] Federal University of Minas Gerais, Department Mechanical Engineering, Belo Horizonte, MG, Brazil, rma@ufmg.br

Abstract – Validation of a numerical simulation based on mathematical model is part of its development and in practice this validation is based on the comparison with experiments. However, the uncertainty of experiment and numerical simulation has not yet received any attention. Generally, only a qualitative assessment of the numerical simulation is provided. Knowledge of the uncertainty is required in order to compare the results since it allows users of the result to assess its reliability. This paper emphasizes numerical simulation components uncertainties. A procedure is adopted to validation of numerical simulation considering the uncertainties and an illustrative calculation will be discussed.

Keywords: Validation; Measurement Uncertainty; Numerical Simulation Uncertainty

1. INTRODUCTION

In recent years, considerable attention has been concentrated on developing sophisticated models capable of predicting various processes. The development of numerical methods for modeling these processes is helpful in designing and controlling processes in order to achieve better quality products. Numerical simulation based on valid mathematical models offers opportunities to gain insights into various physical phenomena that are difficult, if not impossible, to extract through experiments. Thus, modeling becomes more attractive for exploring novel processing schemes. However, in carrying out this development it is necessary to know if the complete numerical model, governing equations, boundary conditions and numerical solutions are a reasonable representation of the physical reality. Furthermore, if the numerical solution scheme accurately solves the governing equations [1-2].

The first of these questions involves the comparison with experiments, process measurements and to some extent physical intuition. Answering the second question is a large problem in numerical analysis. A direct way of accessing the accuracy of a given numerical scheme is to compare predictions against test solutions, i.e. analytical, semi-analytical or approximated solutions of limiting cases of the model. A weakness in this approach is that these limiting models may be far removed from the system of interest. Also, in some cases, due to the high costs, available experiment data are very limited and therefore there is no measure correspondence with any data model. This means that we can say only that it is good, bad, etc. These are sometimes preliminary analysis that can be useful as a guide for the next set of analysis, but it is exceedingly dangerous to base any design decisions on them [3-4].

The terms verification and validation are frequently found in literature and apparently seem to be easily understood intuitively. However, in practice these terms are source of confusion. Verification is a process to check the correctness of the solution of the governing equations. Verification does not imply that the governing equations are appropriate; only that the equations are being solved correctly. Validation is a process to determine the appropriateness of the governing equations as a mathematical model of the physical phenomena of interest. Typically, validation involves comparing model results with experimental measurements. However, some of the works only provide a qualitative assessment of the model, concluding that the model agreement with a particular experiment is good or reasonable. Sometimes, the conclusion is that the model works well in certain cases, not as well in others. Moreover, recent reviews of some models have suggested the existence of significant differences between models. Generally the validation takes in count only the difference between the results, without considering the uncertainty of the experiment and neither the uncertainty of the numerical simulation. However, all experiments are subject to imperfections. As well as, in the mathematical model, for example, its construction (e.g., a partial differential equation) involves idealizations and inexactly known values for geometric quantities, parameters and material constants. Some examples of sensitivity studies, which are part of the development model, are provided. Model parameters can be the physical properties, boundary conditions, initial conditions, etc. The parameters can also be purely numerical, like the size of the numerical grid.

The validation must provide the information to address adequacy, before stating whether a given model is validated for its application or not. Before we proceed with the validation process, we have to know the requirements our product or system will have to meet and which ones our model is to address. Thus, it has become evident that to

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establish mutual confidence between the experiment and numerical simulation, it is necessary to estimate their uncertainties. When uncertainty is not taken into account it is not possible to compare two results. Verification and validation contributes directly to the decision process for investment, through quantification of uncertainties at the confidence for margin and reliability assessments. The objective of the current paper is to present a discussion about validation of numerical simulation based on mathematical models. Different components of uncertainties are discussed, with emphasis on numerical simulation components uncertainties.

2. UNCERTAINTY OF NUMERICAL SIMULATION

The uncertainty in the experimental result is calculated on the basis of the uncertainty in the measurements of all the related independent variables. It is usually given as a 95 % level of confidence and would normally be expressed in the appropriate SI units [5]. Detailed descriptions and information on the implementation of this methodology have been published by ISO and made available over the Internet. Fig. 1 shows typical scenarios arising when it is compared results of experiment and numerical simulation based on mathematical model considering the uncertainties.

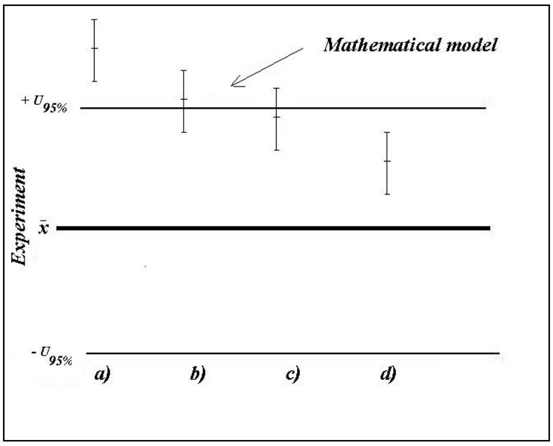

Fig. 1. Comparing of measurement results of experiment and those obtained from mathematical model a) result of mathematical model out of upper limit expanded uncertainty interval of experiment $U_{95\%}$ b) result of mathematical model above upper limit and its expanded uncertainty interval is partially below of upper limit expanded uncertainty interval of experiment c) result of mathematical model below limit and its expanded uncertainty interval is partially below of upper limit and d) results plus expanded uncertainty within expanded uncertainty interval of experiment.

When estimating the uncertainty we must remember that it is neither routine task nor a statistical exercising. Our approach must depend both on a total description and knowledge of the process. The quality and applicability of the uncertainty value depends mostly on understanding, critical analysis, and completeness of all contributing factors. An estimate of uncertainty of numerical simulation model should be based on the combination of a number of components of uncertainty such as uncertainty due to inputs of the models (e.g. physical properties, boundary conditions, initial conditions, etc), numerical procedure (e.g. mesh test and numerical scheme) and simplifying assumptions. Some of these components are well defined and evaluated while others are based on varying degrees of knowledge and experience. All factors which will have a significant influence on the test must be included in the estimation process.

a) Model inputs

The point has been reached where, if appropriate input quantities/data are employed, one can be reasonably confident in the quality of the model represented by governing transport equations. The input quantities of a model are of two categories: those that are submodelled as functions of other quantities; and those that are not modeled. In many cases these quantities are in the form of a table, say in a handbook of material properties. The best estimate of a quantity is then, simply, the value read from the table. In general, the entries in the table will have been established empirically, on the basis of experiments carried out elsewhere. However, rarely, if ever, will those values be given together with their corresponding uncertainties. In the absence of specific information on this matter, the user may use his/her judgement to set a maximum error for the values in the table. To estimate a value of this quantity, one has to consider factors such as the presumed difficulty in the measurement, the year in which the table was made, the reliability of the source, the values of the same quantity tabulated in other handbooks, etc [6].

b) Numerical procedure

Every numerical method has a set of problems for which it is valid. Sometimes you can prove that a certain problem is not in that set but you cannot prove that it belongs to the set. Thus, all numerical approximation schemes are prone to a degree of error. Some errors are a result of truncation of additional terms in series expansions. Others are a result of the order of the differencing scheme used for the approximation. There are a number of ways in which a differential equation can be converted into its discrete counterpart. For example, an analytical solution consists of an expression for T (temperature) in terms of x. The numerical solution, by contrast, is given in the form of the numerical values of T at a finite number of locations (grid points). The discrete values of T are governed by algebraic equations, which we call discretization equations. When only a small number of grid points are used to discretize the calculation domain, the discretization equations represent an approximation to the differential equation. This approach involves discretizing the spatial domain into finite control volumes using a mesh. Then, the resulting numerical solution would normally not coincide with the exact solution of the differential equation. As we increase the number of grid points, the numerical solution becomes more accurate and approaches the exact solution. For many problems, even a modest number of grid points can lead to solutions that are sufficiently accurate for practical purposes. Furthermore, for many problems for which exact analytical solutions may not be available, we can treat the numerical solution as sufficiently accurate when a further increase in the number of grid points does not alter the solution. In general, the finer the numerical grid, the better the numerical solutions of the equations. However, because of the non-linearity of the equations, the decrease in discretization error does not necessarily translate into a comparable decrease in the discretization error. To find out what effect a finer grid has on the solution, model users usually perform some form of grid sensitivity study in which the numerical grid is systematically refined until the output quantities do not change appreciably with each refinement. Thus, there are errors due to an unsuitable selection of numerical method and numerical errors within the selected numerical method.

c) Assumptions

Several assumptions are typically introduced to simplify the solution of the conservation equations. There are always phenomena that we have decided not to include in the model. Applications of these assumptions have confirmed important features that were previously observed but had eluded prediction. Moreover, there are various formulations for the same assumption. It is interesting to examine the differences between the alternative formulations and to investigate how the predictions change when alternative formulations are employed. Some of these assumptions might be found to be negligible, while others could be substantial, depending on various factors including the nature of the assumption being investigated. Each of these assumptions can be further separated into very specific factors, depending on their needs and the applications. To estimate the effect of these assumptions added/subtracted terms in the equations. In general in order to better evaluate and understand models, the effects of these assumptions on the resulting model predictions need to be investigated.

3. VALIDATION OF NUMERICAL SIMULATION

The quality and applicability of the uncertainty value depends mostly on understanding, critical analysis, and completeness of all contributing factors of numerical simulation. It is best if the experiment is designed purely to validate a model, in which case one can eliminate error sources by simplifying the geometry and materials. For its evaluation it is proposed the following plan.

Step1: To verify that the equations are not violating fundamental laws like conservation of matter and energy.

Step 2: To describe the variables, parameters, formulations assumptions and interrelationships between those. To inform all types of numerical errors and modeling errors. To identify uncertainty sources. Concentrate efforts on significant sources of uncertainty.

Step 3: To get two sets of data that cover the whole range of the values found. Also, do it for alternatives formulations and assumptions. It is important to show the origins of its data for comparison.

Step 4: Calculate the maximum difference between the measured and predicted values and standard uncertainty for each component.

Step 5: Compare each result with respect to the stated uncertainty the results of experiment.

4. ILLUSTRATIVE EXAMPLE

In order to illustrate the validation of numerical simulation results of different simulations were compared to assess the effect of including different approach and data in the calculation of freezing point of zinc. Comparison has been made between predictions obtained when using different formulations/data that are available in the literature. For our purposes, the most important sources of uncertainty are due to interfacial area concentration, drag interaction term, permeability coefficient, mesh test, thermophysical properties (specific heat, thermal conductivity and latent heat) and partition equilibrium coefficient [7].

The simulated geometry is shown in Fig. 2. The size was selected to be representative of a laboratory cell where the melt is placed in a cylindrical graphite crucible; a hole in a removable graphite top allows a graphite thermometer well to be axially located in the melt. The symmetry of the cell allows a ¼ section of the geometry to be modelled. The top, bottom and the left wall of geometry the cell are insulated while a temperature is prescribed at the right wall (the crucible external radius). All walls are treated with a no-slip condition and are impermeable to mass and species transport. The melt is initially isothermal and chemically homogeneous. In all simulations presented in this paper the initial temperature was 5 K higher than the liquidus temperature. At time $t = 0$, the temperature of the crucible external radius was altered to 692,677 K and it was reduced with a freezing rate at about 0,01 K/s. The interfacial length scale was assumed equal 0,2 mm and diffusion lenghts for all species are assumed equal 0,01 mm. These quantities are constants and assumed to be representantive of those found in literature for zinc point. The freezing curves were deduced from temperature in the themometer-well, where the sensing element of the thermometer is axially located.

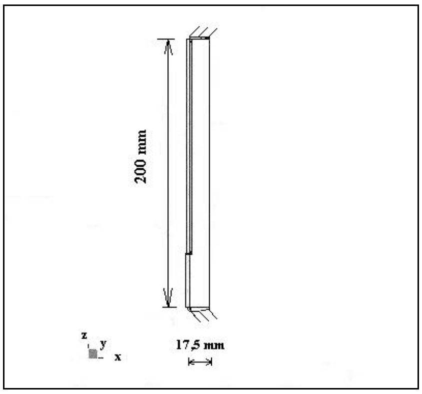

Fig. 2. Geometry of cell zinc point.

a) Interfacial area concentration

The interfacial area concentration characterizes the topology of the interfacial structures and is thus related to complex microscopic phenomena. It plays important roles in the modeling of the interfacial terms and need to be modeled through supplementary relations, which can be developed from either experiments or certain theoretical concentrations. Two cases were investigated, the mixture model and envelope dendrite model. The mixture model is a model that treats both phases symmetrically. It is appropriate as a first approximation for more complex problems [8]. In the dendrite envelope model the area concentration is modeled as equivalent cylinders. These are most appropriated for the columnar growth [9].

b) Drag interaction term

Flow through a mushy zone consisting of a continuous solid structure such as columnar dendritic crystals is usually very slow due to the high value of the interfacial area concentration. Firstly, the dissipative interfacial stress was modeled approximately by Darcy's law [10]. In addition, the permeability was converted into a drag coefficient [11]. The modeling of this term requires experimental calibration to link the drag coefficient to microstructural parameters. However, a generalized expression was used to estimate this term (Fig. 3).

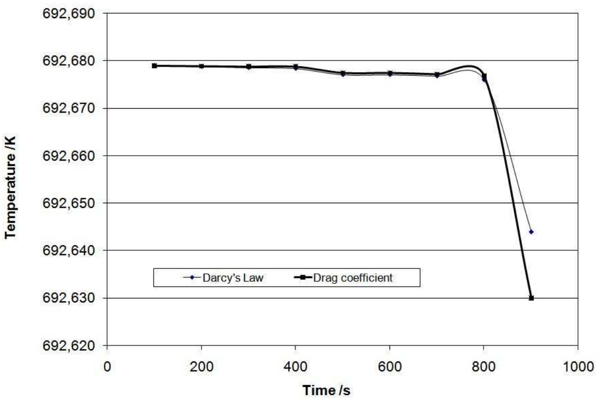

Fig. 3. Drag interaction term effect.

c) Permeability coefficient

The permeability coefficient contains the interfacial area concentration implicitly. Assuming the permeability to be isotropic, it was evaluated from the Blake-Koseny model. This value is based on experimental measurements for low liquid fractions and is based on analytical solutions for flow through arrays of high liquid fractions. This model has been used extensively in solidification simulations with constant permeability. Since permeability coefficient of dendritic structures is typically of the order of 10^{-10} m^2 to 10^{-14} m^2 ten simulations were run with these values (Fig. 4) [7].

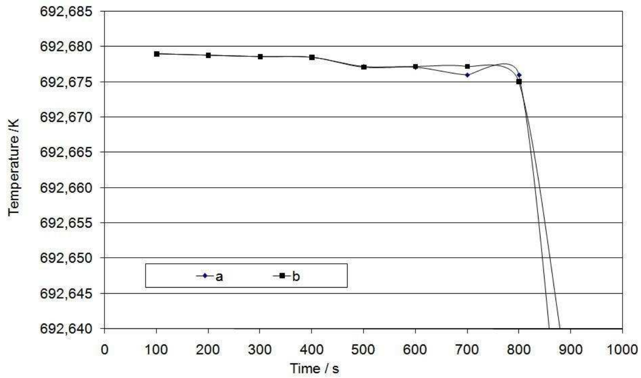

Fig. 4. Permeability coefficient effect a) $C_o = 10^{-10}$ m^2 b) $C_o = 10^{-14}$ m^2.

d) Mesh test

Often, the first step after the development of the model is the mesh test. This test is used to refine the surface and volume mesh in regions of model, generating progressively finer elements. At the end of each run, the results were compared. The final mesh was selected when the difference between the results of two successive curves of solidification was lesser than experiment uncertainty measurement. The final mesh contains 48 994 tetrahedrons elements. The bulk of the geometry contains total number of 9 990 nodes (Fig. 5).

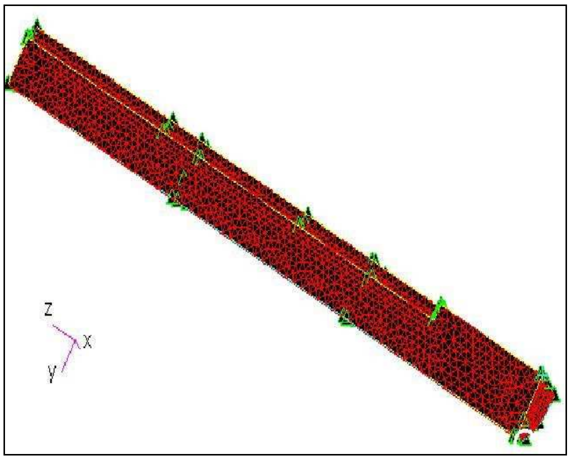

Fig. 5. Red triangular surface mesh covering the surface of the geometry.

e) Thermophysical properties/partition coefficient

Two different predicted curves of solidification, using two sets of data from the literature were compared [7]. Results of the solidification using different partition coefficients illustrated that the model is extremely sensitive to the specification of this parameter. The magnitude of difference for the other cases (thermophysical properties) was lesser than experiment measurement uncertainty.

4. RESULTS

The results of the evaluation of numerical simulation are summarized in Table 1. The estimates for the influence of each component were deduced from the maximum difference between the results. The magnitude of difference varies from 0,1 mK to 0,6 mK with standard uncertainty from 0,02 mK to 0,17 mK. The uncertainty due to experiment is 1 mK, which is higher than standard uncertainty of each component. Taken all together, the present results should be viewed as an indication of what areas require more careful examination.

Table 1. Maximum difference between experiment and numerical simulation.

Components	Maximum difference /mK	Standard uncertainty /mK
Interfacial area	0,6	0,17
Drag interaction term	0,4	0,11
Permeability coefficient	0,1	0,02
Mesh test	0,6	0,17
Thermophysical properties	0,6	0,17

5. CONCLUSIONS

Sufficient evaluation of numerical simulation based on mathematical models is necessary to ensure that those using the models can judge the adequacy of their technical basis, appropriateness of their desired use, and confidence level of their predictions. Most validation exercises are done simply to assess whether or not the model can be used for a very specific purpose. In general, the validation of numerical simulation is based on comparison with experiments. A weakness of this procedure is not to considering the uncertainty of experiment and numerical simulation. The result of an experiment or a numerical simulation is the estimate of the true value of the measurand. Thus, the result is imperfect. We have shown that it is possible to estimate the uncertainty of a numerical simulation. In this case, the estimation of uncertainty of numerical simulation is based on the combination of a number of influencing parameters (components of uncertainty) obtained from various predictions. Some of these components are well defined and evaluated, while others are based on varying degrees of knowledge and experience. A formal and rigorous evaluation is time consuming and expensive. The present results show that the standard deviation of each component is lower than uncertainty due to experiment, so there is a scope for further improvement in the model by refining the assumptions.

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