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NON-DESTRUCTIVE TESTING

RECOMMENDATIONS FOR THE USE AND VALIDATION OF NON-DESTRUCTIVE TESTING SIMULATION

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IIW COMMISSION V

NON-DESTRUCTIVE TESTING AND QUALITY ASSURANCE OF WELDED PRODUCTS

Commission V

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Non-destructive Testing and Quality Assurance of Welded Products

IIW Commission V, chaired by Dr. Eric Sjerve (IrisNDT, Canada)
Author: Dr. Pierre Calmon (CEA, France)

Recommendations

for the use and validation

OF NON-DESTRUCTIVE TESTING SIMULATION

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RECOMMENDATIONS
for the use and validation of non-destructive testing simulation

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1. INTRODUCTION

Numerical simulation (also called "theoretical modelling" or "computer modelling") is a powerful tool being used increasingly in the NDT field. The reliability of any conclusions drawn from simulation depends directly on the validity of the codes and models used. The main objective of this document is to give advice and recommendations on procedures for the validation of codes and models. The aim is to promote a uniform approach for the validation of NDT simulation, one aspect being the creation of a validation database.
The document is organized as follows. In the first part we give a brief overview of the different approaches, advantages and limitations of the application of NDT numerical simulation. Then we list some considerations and recommendations for the use of simulation. In the second part of the document we discuss the different aspects of validation and give recommendations on both validation procedures and reporting of validation data. The key point here is that the model user should be able to cite validation data demonstrating the relevance and reliability of the code being used.

About the author:

Pierre Calmon received in 1990 the PhD in Physics at the University of Paris Sud, France and joined the NDE department of the French Atomic Energy Commission (CEA). Since then his research activity has been mainly focused on modeling and simulation. Initially involved in the development of NDT simulation software he is now responsible of coordinating the research in NDT at CEA. He is the current Chair of IIW Commission V-F "Reliability of NDT".

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2. CONSIDERATIONS AND RECOMMENDATIONS ON THE USE OF NDT SIMULATION

2.1 Scope and definitions

NDT simulation is used nowadays in a wide range of different applications:

- Performance demonstration of existing method
- Reliability assessment of method through Probability of Detection (POD) studies
- Study of the inspectability of components through "virtual" testing
- Help in analysis, better understanding of underlying phenomena, data inversion
- ...

In general, the application of simulation is aimed at technically justifying the use of one technique, one probe, one data processing algorithm, etc… in relation to the final objective being pursued by the practitioner. In such cases the information provided by simulation is included as an element of the technical justification.

By simulation we mean the use of a software program providing quantitative predictions on some aspect of the inspection process. The software results from the implementation of a numerical algorithm solving a mathematical formulation of the physical phenomena involved in the simulation. We will call "model" the mathematical formulation plus the numerical algorithm.

2.2 Typical ways of using simulation as element of technical justification

In general, NDT techniques consist of measuring the response of the interrogated component or part to an excitation. The excitation is a transmission of energy which interacts with the component and induces the response.
One common use of simulation consists of computing the response of the inspected component (echoes for ultrasonics, variation of impedance for eddy current, etc) after having postulated the presence of one or several flaws whose characteristics are inputs to the simulation.

The computation of the responses of flaws can be used to:

- Predict the signal amplitudes from postulated defects relative to the response of a calibration defect (side drilled hole, flat bottomed hole, etc…)
- Estimate the detection performance of a method as a function of the characteristics of the defect: size and shape, location, material orientation, roughness…For instance simulation can give the minimum detectable size of defect above a given threshold.
- Quantify the influence of various (controlled and uncontrolled) parameters : e.g. the influence of the geometry of the component, the effects of cladding, the effects of metallurgical microstructure, etc.
- Determine a "worst case" among the possible ranges of variation of a set of identified parameters.
- Interpolate between cases covered by experimental data
- Compute POD (probability of detection) curves as a function of the flaw size given a set of varying parameters and their ranges of variation.
- …

A second common practice consists of modelling only the excitation aspect of the inspection (the propagating ultrasonic wave or the induced electromagnetic field in the cases of ultrasonics and eddy currents respectively). In this case simulation gives insight into the capability of the probe to efficiently interrogate the region of interest in the component. Such computation can help in the design or set-up of the probes. In particular beam computations are currently used for designing ultrasonic array techniques.

The simulation of the excitation aspect can be used to:

- Evaluate the sensitivity of a given probe and its set-up
- Better understand the effects of interactions on the defect's responses (for example multiple paths and mode conversions in ultrasonics)
- Better understand the influence of parameters on detection performance (for example the effects of material anisotropy on ultrasonic beams)
- ...

2.3 Main advantages of simulation

- Speed and cost.
- Versatility of the investigated situations: the possibility of considerably increasing the amount of available data and increasing the range of essential parameters investigated (including cross-variations of parameters) by increasing the number of "numerical experiments".
- Explanation of results: the possibility of physically understanding the data provided by simulation either through specific processing functionalities (snapshots of propagating waves for example) or by conducting specific "academic" calculations.

2.4 Different types of simulation tools

A simulation code is defined by the following aspects:

- **Its function** (calculation of ultrasonic wave fields, echoes from postulated defects…) and its regime of application: the NDT technique and the situations addressed by the code and the principal outputs of the code.
- **The theoretical model** on which the calculations are based. In general one simulation can call up several inter-connected models dedicated to the different phenomena involved in the inspection (with the output of one model becoming the input to the next one). In such cases the global model is often described as an "integrated model".
- **The software implementation**.

A wide range of different types of codes may be encountered:

Concerning the function:

- Some codes aim at fully simulating the inspection: the input of the code corresponds to the main essential parameters of the inspection and the main output corresponds to the result of the inspection.
- Some codes are dedicated to one partial aspect of the inspection: e.g. the computation of the excitation field in the component; the calculation of reflection coefficients; the homogenization of a heterogeneous or composite structure and the determination of corresponding effective parameters (attenuation, permittivity, etc…)

Concerning the model it is customary to distinguish between:

- "Analytical models" which calculate analytical expressions giving the solution of the physical problem under consideration. In general analytical solutions are available only for canonical and the simplest situations, so these models generally only address a partial aspect of the inspection.

- "Semi-analytical" models which aim at (numerically) calculating expressions derived from the exact formulation of the problem. These derived expressions (in general integral formulations) use known analytical partial solutions (such as Green's functions) and are often established using some specific approximations.
- "Full numerical methods": Numerical solution of an equation corresponding to a mathematical formulation of the physical problem under consideration and based on spatially or temporally sampling the elements of the inspection (probe, medium of propagation, defect, etc…). Finite element methods and finite difference methods are the most common methods in this class.
- "Hybrid models" which combine the previous approaches in some way. In general, such methods are proposed with the aim of reducing the size of the sampled region.
- Stochastic models, as opposed to deterministic models, are based on algorithms using random processes.

Concerning the software implementation one can distinguish between:

- NDT oriented "home-made" codes developed by the end-user institution.
- Commercial packages dedicated to NDT.
- Generalist (commercial or home-made) packages, such as a finite element package which may be applied to solve an NDT issue.

2.5 Considerations when using simulation

For each of the different situations listed above, there are corresponding advantages and disadvantages which need to be evaluated depending on the intended user application. In general the considerations mainly concern:

- **The physical basis of the model**, its domain of applicability and the expected reliability of its predictions. Does the model account for the influence of the essential parameters of the inspection? Is it a 2D or a 3D model? Has it already been used or validated in the context of similar applications? etc …
- **The computer resources** required to run the code and the **numerical performance** in terms of computation time.
- **The personnel competence** required to run the code. Is specific skill in numerical techniques required to set up a simulation and interpret the output?

2.6 Recommendations when using simulation

The crucial issue when using simulation is to evaluate the level of reliability of the predictions furnished by the code. Great care must be given to the relevance of the computations by considering the physical basis of the model and the domain of applicability of the code. This is especially true since simulation software codes are powerful tools offering multiple possibilities and are based on sophisticated mathematical and numerical theories.

To allow a reasonable evaluation of the credence that can be given to simulated results, it is recommended that the following information is included when reporting these results:

- The name of the code, the organization which developed it, and the version number which has been used. The reliability of a computation depends not only on the validity of the underlying theoretical model but also on the correctness of the software implementation. The identification of the version number is absolutely essential to clearly establish this correctness (lack of critical bugs).
- The inputs to the code:
  - ⇒ A list of the principal inputs to the code and their correspondence to the identified essential parameters of the inspection. The establishment of this correspondence may help with checking what aspects are taken into account by the code. (It should be noted, however, that just because an input is entered by the user it does not follow that this input is correctly taken into account by the code).
  - ⇒ The values assumed for these parameters in the inputs corresponding to the carried out simulations.

- The different elements justifying the relevance of the code:
  ⇒ Consideration of the physical basis of the model and its domain of validity: engineering understanding and theoretical considerations.
  ⇒ Available and controlled data related to the validation of the model or the code in similar situations: data from the literature, international benchmarks, experimental databases etc...
  ⇒ Experiments carried out specifically with the aim of evaluating the reliability and accuracy of the code in the case under study.

3. CONSIDERATIONS AND RECOMMENDATIONS FOR THE VALIDATION OF CODES

3.1 Scope and definitions

As emphasized above, the availability of validation data is a key point when using NDT simulation.
By the validation of one code or one model we mean the process of evaluating the reliability/accuracy of its predictions by comparing these predictions to reference results. In general these are obtained by experiment (experimental validation), but they may also be obtained using other codes or models (model benchmarking, which will be called "numerical" validation here). The notion of reliability/accuracy and consequently the means of evaluating it will be clarified in the next sections.

3.2 Considerations on accuracy and uncertainties in the context of validation

3.2.1 Possible origins of discrepancy between experiment and simulation

Firstly we note that it is somewhat simplistic to regard experiments as providing "true" values which have to be reproduced as closely as possible by simulation. Uncertainty in the essential parameters and the accuracy of the experiment itself also have to be considered. Therefore discrepancies between experimental and simulated results cannot automatically be taken as a direct measure of the accuracy of the simulation.

The discrepancy between one experimental result and the corresponding simulated result may be due to:

1. Experimental uncertainity
2. Inaccuracy of the representation of the real trial by the inputs of the simulation
3. Numerical uncertainties (numerical noise and the influence of computational parameters)
4. Inaccuracy of the model (approximations)
5. Bugs in its implementation

The final goal of the validation is to quantitatively determine the component of the discrepancy actually due to the simulation itself. Such evaluation constitutes a measure of the "reliability" of the simulation. As discussed in §3.4, the regime of validity of the process under validation may vary depending on the objective pursued by the NDT practitioner.

3.2.2 Scope of the validation

We can distinguish between somewhat different situations:

- When the objective is to test the capability of the code to reproduce experiment for one given application specified in one material (identification of the equipment and inspected component), the process under validation includes the simulation plus the representation of the reality in terms of qualifying characteristics and essential parameters.

The sources of error in the above list which must be considered as possibly contributing to the inaccuracy of the "simulation" are items 2 to 5.

This situation corresponds to the least informative one. The conclusions of the validation are essentially limited to the application under consideration.

- When the objective is to evaluate the reliability of the predictions provided by one given code in a range of situations of interest defined by qualifying characteristics (on probes, components, flaws…), the process under validation is reduced to the simulation itself.

The sources of error in the above list which must be considered as possibly contributing to the inaccuracy of the "simulation" are items 3 to 5.

In this case the conclusions of the validation can be transposed to similar applications of the same code.
When the objective is to evaluate the validity of the theoretical model itself (the mathematical formulation and eventually its numerical implementation) or one limited aspect of the model (one specific approximation), the process under validation is limited to the model.

The sources of error in the above list which must be considered as possibly contributing to the inaccuracy of the "simulation" are reduced to items 3 and 4.

This situation is the most academic and the most general. The information provided is of interest not only for one specific code but can be transposed and help with justifying the use of other simulation codes based on a similar model.

3.2.3 Experimental uncertainity

The accuracy of the experiment itself is measured by the reproducibility of experimental results for one fixed set-up (one fixed equipment, one fixed specimen under test and one fixed procedure). The possible factors limiting the accuracy of the experiment are: sources of noise, fluctuations in parameters pertaining to the measurement, the effects of influential parameters or phenomena not listed in the definition of the set-up.

Recommendations related to this issue are given § 3.4, items 5 and 6.

3.2.4 Uncertainty linked to the determination of the inputs of the simulation

The real trial is represented by an amount of information transformed into inputs for the simulation code.

The inputs of the simulation generally consist of qualifying characteristics (type of probe, isotropy of the material, etc…), and the values of essential parameters (frequency of the excitation, wave speed in the component, CAD files, etc…). In general identifying elements, such as the type or serial number of a piece of equipment, are not part of the information transferred to the simulation.

This representation of the real experiment by a set of inputs:

i. is based on hypotheses about the specimen under test (geometrical assertions, material considerations, etc…) or about the equipment behaviour (piston source behaviour of ultrasonic probes for example),
ii. requires the determination of the input values of the essential parameters.

Both hypotheses which may be approximations, and uncertainties or inaccuracies in the determination of essential parameters, may have a considerable influence on the relevance of the simulated results.
Recommendations related to this issue are given § 3.4, items 4 and 7.

3.2.5 Numerical uncertainities

In a somewhat similar way as for experiments, one must consider the possibility of uncertainty in the simulation corresponding to a possible non-reproducibility of the simulated result for fixed input and output definitions. Such uncertainty is referred to as "numerical noise", and depends on the characteristics of the model (deterministic or stochastic, analytical or numerical etc…). In general it can be neglected, but when this is not the case it is recommended (item 13 of §3.4) that confidence limits associated with the computed values are evaluated.

In addition it should be noted that, in general, running the code also requires the specification of "computational parameters", specific to the implemented algorithm. These computational parameters (for instance meshing parameters) influence the output of the simulation. One might define and measure one inaccuracy of the simulation linked to this issue in reference to the output corresponding to the "ideal" set of such parameters. However, such a concept is not a very useful one considering our objectives. Recommendations related to this issue are given § 3.4, item 12.

3.2.6 Software testing

When it is the simulation code which is under validation, the distinction between bugs and other numerical sources of errors is not required. Nevertheless indications of the existence of bugs ("abnormal" behaviour of the code) must be considered and reported (recommendation 15 of § 3.4.4).
It is only when the validation addresses the model itself or one aspect of the model that it is crucial to be sure that observed discrepancies between computation and results are not due to bugs.
Software tests are outside the scope of this document so we will not give recommendations on this aspect.

3.3 Considerations on accuracy and uncertainties in the context of validation

One partial way to evaluate the reliability of a model or a code (Code1) may be to compare its predictions with the results provided by an independent code (Code2) considered in that test as a reference.

It should be noted that:

- Agreement (within a relevant interval of accuracy) between the results given by the two codes for the same situation is a convincing indication of:
  - ⇒ The correctness of the software implementation of the two codes.
  - ⇒ The validity of the model (mathematical formulation and its resolution by numerical algorithm), but only if the two models considered are different.

- • On the contrary, if different results are obtained with the two codes it is more difficult to draw conclusions, and some precautions must be taken:
  - ⇒ The discrepancy between the two results can be attributed to the approximations of the model or to a bug in implementation in Code 1 only if the validity of Code 2 has been undoubtedly established for the inputted configuration.
  - ⇒ The discrepancy may also be due to differences between the situations considered by the codes. A careful analysis of the inputs of the two codes is necessary before drawing conclusions. Due to possibly different definitions of the parameters inputted to the codes and different adopted conventions this analysis may be difficult. This is especially the case when the results are obtained from the literature.

3.4 Recommendations for the conduct of experimental validation

3.4.1 Scope of the validation

The first step is to define with precision the scope of the validation. Such a definition will determine how to manage the different aspects of the validation (cf. previous discussion of § 3.2.2).

3.4.2 Design of experimental set-ups

The design of experiments, that is the choice or specifications for mock-ups, flaws, probes, experimental procedures, parameter set-ups, etc…, depends on the regime of validity and objective of the validation. Related to this step it is recommended:

1. To consider the representativeness of the tests according to the situations of interest and to the coverage of the range of varying parameters (such as flaw size, angle beams, etc…) under investigation.
2. To simplify the test as far as possible, in order to isolate the phenomena under consideration and to minimize the interference with other factors which might complicate the interpretation of results. For example if the validation concerns only the influence of the defect size or orientation on its response, canonical geometries and isotropic materials are preferred to more complex mock-ups.
3. To prefer probes and mock-ups whose characteristics are controlled and well-known.
4. To consider the validity of any hypotheses assumed about the specimen (geometrical and material properties such as isotropy, homogeneity…).

3.4.3 Experiments

When carrying out experiments and in accordance with the discussion of § 3.2 it is recommended:

5. To list the influential parameters of the experiment, to check that these parameters are well-controlled and to determine their values.
6. To check the reproducibility of the experiment and to evaluate confidence interval of the reported data.
7. To perform the necessary measurements in order to determine or confirm the hypotheses made and the values of the influential parameters which are not directly controlled by the experimentalist and in particular:
   - ⇒ The materials characteristics of the mock-up, such as ultrasonic velocities, sizes and positions of artificial defects, etc…
   - ⇒ The topology of the mock-up (profilometry)
   - ⇒ The characteristics of probes: these are not always available especially when commercial probes are used. Experiments should be performed on the probes to check that the characteristics of the radiated beam (orientation, width, etc…) correspond to the nominal values furnished by the manufacturer.
8. To evaluate the accuracy of these measurements and report the corresponding confidence intervals.

3.4.4 Computations

As already indicated great care should be given to the input/output definition of the code. In particular it is recommended:

9. To check the correspondence between the data (pertaining to the description of the test to be simulated) required as input to the code and the available data experimentally controlled. When there is not a complete correspondence, to identify and report the missing information and the operations performed to complement the data (extrapolation, approximations, signal processing, etc…)
10. To check the correspondence between the output of the code and the data provided by the experiment. When there is not an exact identity, to report the fact. When post-processing operations are performed, either on the computed or on the experimental data, to report these operations.
11. To perform computations in order to evaluate the inaccuracy caused by uncertainties in the essential parameters. For example, simulation should be carried out for the maximum and minimum values of the uncertain parameters in at least one representative case.
12. To list the computational parameters (inputs which do not pertain to the description of the experiment) and to check the correctness of the specified values.
13. When necessary, to perform tests on the influence of these computational parameters, on at least one representative computation. It is common that one or several parameters drive the accuracy of the computation. In such cases the recommended practice if possible is:
    - ⇒ To increase successively the level of precision of the computation until convergence of the output is reached within a pre-defined interval.
    - ⇒ If this convergence is reached using acceptable computer resources and computation time, then the corresponding value of the computation parameter is adopted for the complete set of computations.
    - ⇒ If this is not the case, the corresponding uncertainty in the output is reported as a measure of the accuracy of the simulation.
    - ⇒ In all cases the values of the computational parameters should be reported.
14. When necessary, to evaluate the reproducibility of the computation and report the amplitude of the "numerical noise".
15. To report "abnormal" behaviour of the code in regards to engineering understanding. This may indicate the presence of bugs or inadequate usage of the code.

3.4.5 Comparisons between experiment and computation

The comparison aims at isolating the part of the discrepancy effectively due to the process under validation (the "simulation"). As already discussed in § 3.2.2, the regime of validity of the "simulation" depends on the exact objective of the NDT practitioner and we can distinguish different situations:

16. When the process under validation includes the simulation plus the representation of reality in terms of qualifying characteristics and essential parameters (that is when the objective is to test the capability of the code to reproduce experimental results for one given application):
    ☞ The discrepancy between the simulated data and the experimental data should be compared to the confidence interval of the experimental data.
17. When the process under validation is reduced to the simulation stricto sensu (when the objective is to evaluate the reliability of the predictions provided by one given code in a range of situations of interest defined by qualifying characteristics (on probes, parts, flaws,…) and values of essential parameters):
    ☞ The discrepancy between the simulated data and the experimental data should be compared to the confidence interval resulting from uncertainty in the experimental data plus the uncertainties in the representation of reality in terms of inputs.
18. When the objective is to evaluate the validity of the model itself (the mathematical formulation and its numerical resolution) or one limited aspect of the model (one specific approximation):
    ☞ The discrepancy between the simulated data and the experimental data should be compared to the confidence interval resulting from uncertainty in the experimental data, plus the uncertainties in the representation of reality in terms of inputs, plus the numerical uncertainties (noise and the influence of computational parameters).

4. RECOMMENDATIONS FOR INCLUSION IN VALIDATION DATABASE

4.1 Inclusion of experimental data in a validation database

In this section we consider the inclusion of experimental data in the database. Since the aim here is to make possible the future use by the NDT community of this data for validating various codes or models, the information provided must be the most comprehensive possible within any limits imposed by confidentiality considerations.

Ideally, the information includes:

- The identification (type) of the acquisition equipment constituted by the excitation and reception devices and including transducers, probes, detectors…
- The set-up of the acquisition parameters
- A report of measurements carried out in order to determine probe characteristics (orientation and focal width of ultrasonic beams, transmitted signals, etc…)
- A description of the specimen under test: constitutive materials (and possibly microstructure), geometry, included flaws (location, size, profiles…)
- A report of the measurements carried out to characterize the specimen (measurements of wave velocity, attenuation, size of defects, etc…)
- A definition of the experimental procedure: probe positioning and scanning, stored signals, reported parameters, any signal processing performed, operations of calibration (characteristics of the reference blocks)
- The post-processing of the results
- The accuracy of the experimental data (reproducibility of the result)

4.2 Inclusion of comparison results in a validation database

The inclusion of validation data (reporting of a comparison between one code or one model and experimental data) may be helpful if it is accompanied by a comprehensive description of the experiment and simulation carried out. The information includes:

- The exact objective of the validation: evaluation of the capability of one code on a given situation, validation of one code in a range of situations, of one model or one approximation.
- The experimental data and the associated information following the prescription of § 4.1.
- The identification of the software: name of the code, organization which developed it, and version number which has been used.
- A general description of the model: expected regime of validity (what aspects of the inspection are modelled), physical principle, hypotheses and approximations.
- A list of the main inputs of the code and their correspondence to the identified essential parameters of the inspection.
- A list of computations made and the corresponding model inputs: values of the parameters, description of CAD files etc… If the code is publicly available and if it is technically possible, it may be valuable to include input files in the database. This can allow different users to repeat the computations.

- A report of tests concerning i) measurement of the inaccuracy caused by uncertainties in the essential parameters (recommendation 11 of § 3.4.4), ii) the influence of the computational parameters (recommendation 13 of § 3.4.4), iii) measurement of numerical noise (recommendation 13 of § 3.4.4).

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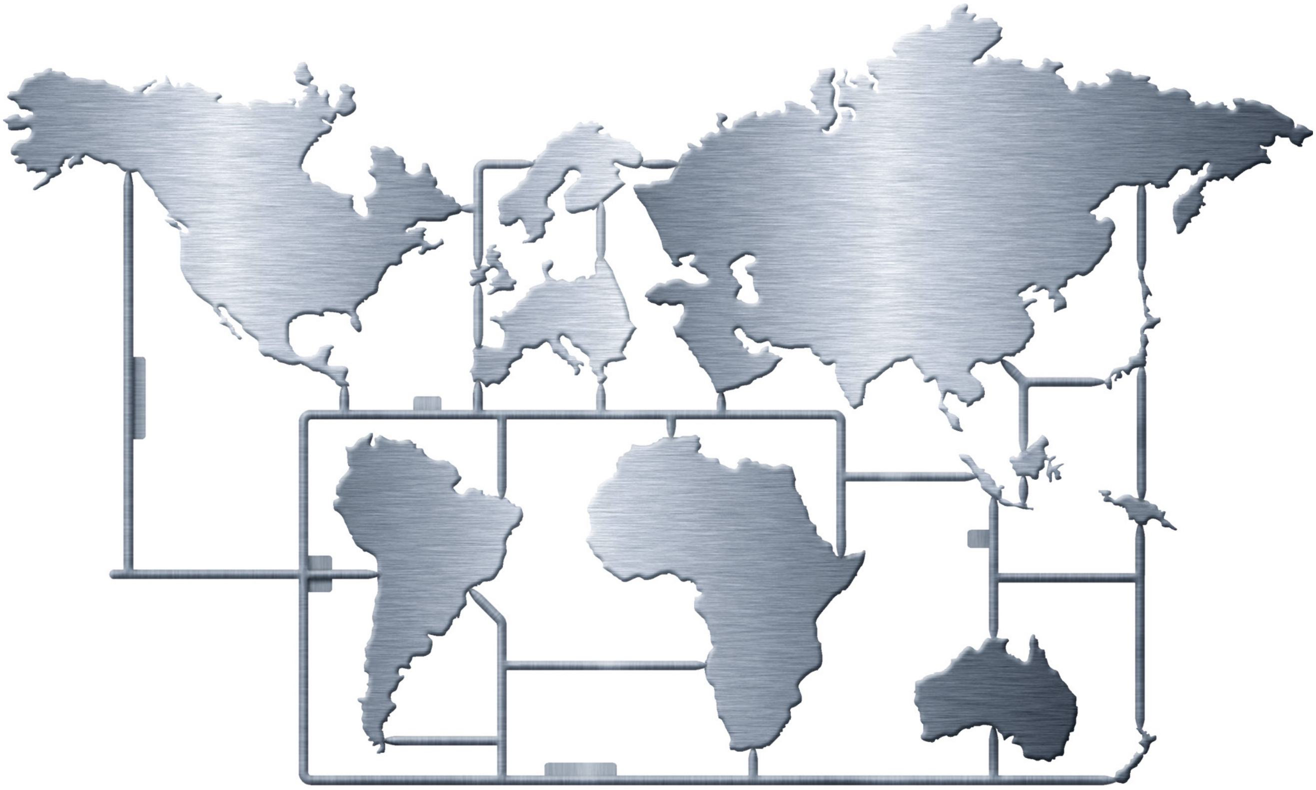

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International Institute of Welding
Office Address :
Paris Nord 2
90, rue des Vanesses - 93420 Villepinte - France
Postal Address :
BP 51362 - Roissy Charles de Gaulle Cedex - France
Fax : +33 1 4990 3680 - E-mail : iiw@iiwelding.org
Website : www.iiwelding.org

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KEYWORDS
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