NEA/CSNI/R(95)23
Supplement

OECD
NEA

AHMED Code Comparison Exercise

Comparison Report

(Revised MACRES Calculations)

July 1996

COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS
OECD NUCLEAR ENERGY AGENCY
Le Seine Saint Germain - 12, Boulevard des Iles
F-92130 Issy-les-Moulineaux (France)
Tel. (33-1)45 24 82 00 Fax (33-1)45 24 11 10

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ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

Pursuant to Article 1 of the Convention signed in Paris on 14th December 1960, and which came into force on 30th September 1961, the Organisation for Economic Co-operation and Development (OECD) shall promote policies designed:

- to achieve the highest sustainable economic growth and employment and a rising standard of living in Member countries, while maintaining financial stability, and thus to contribute to the development of the world economy;
- to contribute to sound economic expansion in Member as well as non-member countries in the process of economic development; and
- to contribute to the expansion of world trade on a multilateral, non-discriminatory basis in accordance with international obligations.

The original Member countries of the OECD are Austria, Belgium, Canada, Denmark, France, Germany, Greece, Iceland, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The following countries became Members subsequently through accession at the dates indicated hereafter: Japan (28th April 1964), Finland ((28th January 1969), Australia (7th June 1971), New Zealand (29th May 1973), Mexico (18th May 1994), the Czech Republic (21st December 1995) and Hungary (7th May 1996). The Commission of the European Communities takes part in the work of the OECD (Article 13 of the OECD Convention).

NUCLEAR ENERGY AGENCY

The OECD Nuclear Energy Agency (NEA) was established on 1st February 1958 under the name of the OEEC European Nuclear Energy Agency. NEA membership today consists of all European Member countries of OECD as well as Australia, Canada, the Czech Republic, Hungary, Japan, the Republic of Korea, Mexico and the United States. The Commission of the European Communities takes part in the work of the Agency.

The primary objective of NEA is to promote co-operation among the governments of its participating countries in furthering the development of nuclear power as a safe, environmentally acceptable and economic energy source.

NEA works in close collaboration with the International Atomic Energy Agency (IAEA), with which it has concluded a Co-operation Agreement, as well as with other international organisations in the nuclear field.

COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

The NEA Committee on the Safety of Nuclear Installations (CSNI) is an international committee made up of scientists and engineers. It was set up in 1973 to develop and coordinate the activities of the OECD Nuclear Energy Agency concerning the technical aspects of the design, construction and operation of nuclear installations insofar as they affect the safety of such installations. The Committee's purpose is to foster international co-operation in nuclear safety amongst the OECD Member countries.

FOREWORD

The NEA Committee on the Safety of Nuclear Installations (CSNI) sponsored in 1994/1995 a code comparison exercise based on NaOH tests performed in VTT's AHMED (Aerosol and Heat Transfer MEasurement Device) facility with the objective of testing containment aerosol codes in well defined conditions prior to an International Standard Problem based on the VANAM M3 test (ISP-37) where aerosol behaviour has been studied in a large scale multicompartment facility. For the code users it was indeed important to know how well codes could predict experimental results in AHMED's well defined conditions before the codes were compared with aerosol behaviour measured in large scale facilities where driving forces were merely thermal-hydraulic. In other words, the codes had to be able to follow the aerosol behaviour in the AHMED facility before they were used in more complex geometries and non-homogeneous thermal-hydraulic conditions.

Six codes participated in the AHMED Code Comparison Exercise. The results were published in the series of CSNI Reports, under the reference NEA/CSNI/R(95)23 (October 1995).

The code MACRES, developed by Japan's Nuclear Power Engineering Corporation (NUPEC), participated in the Exercise. Calculation results for low humidity cases were obviously unrealistic while results for high humidity cases were good. It was reasonable to assume that the code contained an error, or that some calculations were based on wrong assumptions.

As a direct result of the AHMED Code Comparison Exercise, MACRES has been improved. A brief explanation for the changes made by NUPEC is given in the following section, with the results of revised calculations. These new results modify the Discussion and Conclusions based on the initial exercise [Chapter 7 of NEA/CSNI/R(95)23]. A revised 'Discussion and Conclusions' chapter has been prepared by Dr. J. Jokiniemi (VTT), Chairman of the AHMED Code Comparison Exercise.

The improved MACRES code has performed very well in the ISP-37 Exercise.

The attached report is published as an Addendum to CSNI Report NEA/CSNI/R(95)23.

EXPLANATION FOR CHANGES MADE IN MACRES
(prepared by NUPEC)

As a result of the AHMED Code Comparison Exercise, NUPEC reviewed MACRES and came to the conclusion that the poor calculational results in low humidity cases were due to a defect in the code, that is inappropriate modeling, and code bugs. In the AHMED Exercise, NUPEC's reasoning had been the following: Modified Raoult's Law with constant van't Hoff coefficient was thought to not be able to simulate the starting phase of steam condensation on aerosols and that model was thought to affect aerosol size distributions although the time necessary for equilibrium was very small. In order to simulate the starting phase, that is, realistic estimation of water activity at the beginning of condensation, a new approach based on dissolution heat was applied for the modeling. After the starting phase of steam condensation, modified Raoult's Law with constant van't Hoff coefficient was used. The new approach based on dissolution heat was found to not adequately predict water activity and was subsequently removed following the AHMED Exercise.

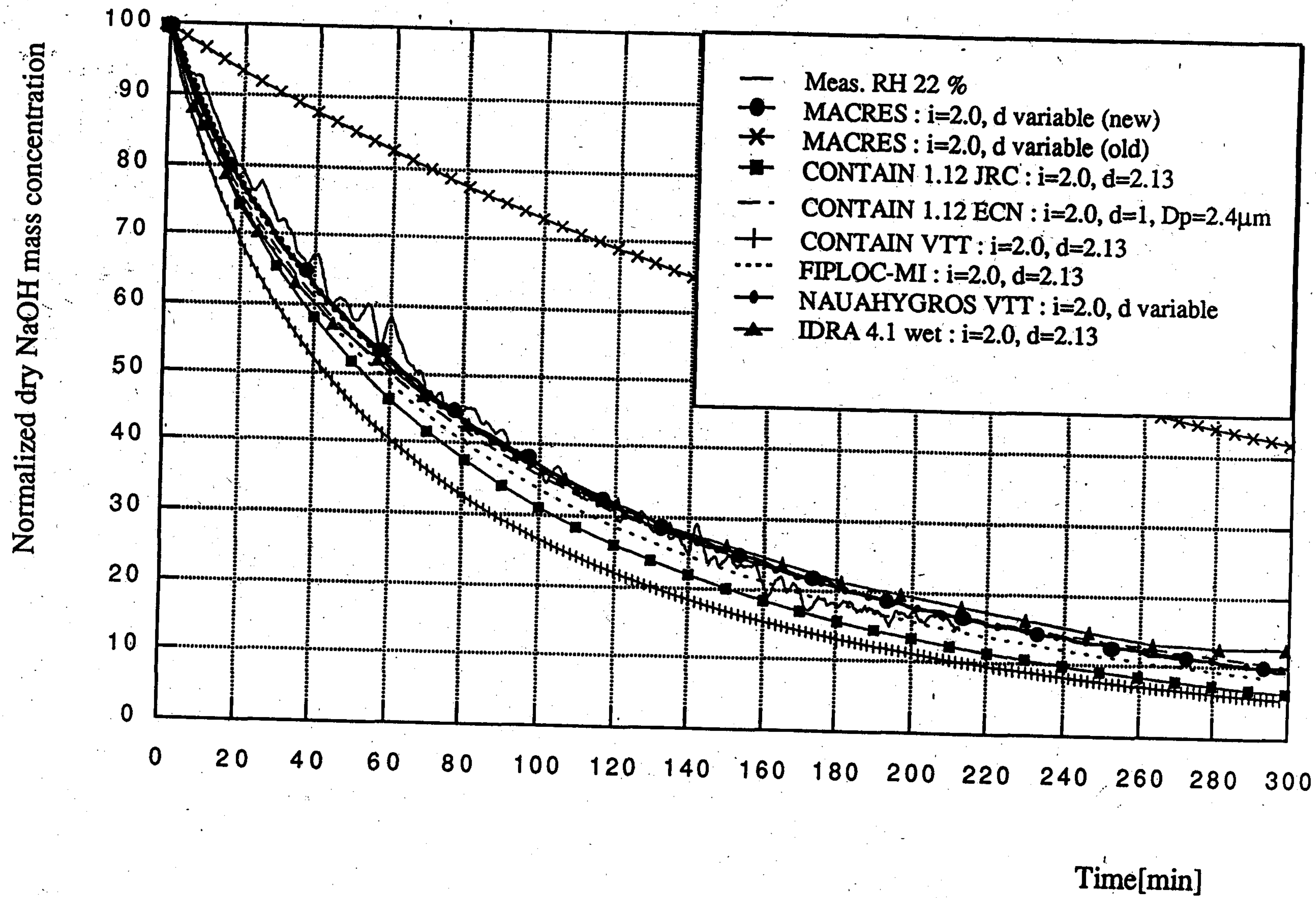
NUPEC's calculational results for the AHMED Exercise were very different from the test results in the low humidity cases while the agreement was good in high humidity cases. Nevertheless, NUPEC submitted all their original calculational results because they thought that it was not meaningless to show the calculations which had been made with the above mentioned model.

After correcting some bugs and incorporating a hygroscopic model similar to those used in other codes, the MACRES calculations have now come to fairly good agreement with the experimental results. The revised calculation results have been plotted on the attached graphs, taken from CSNI Report NEA/CSNI/R(95)23.

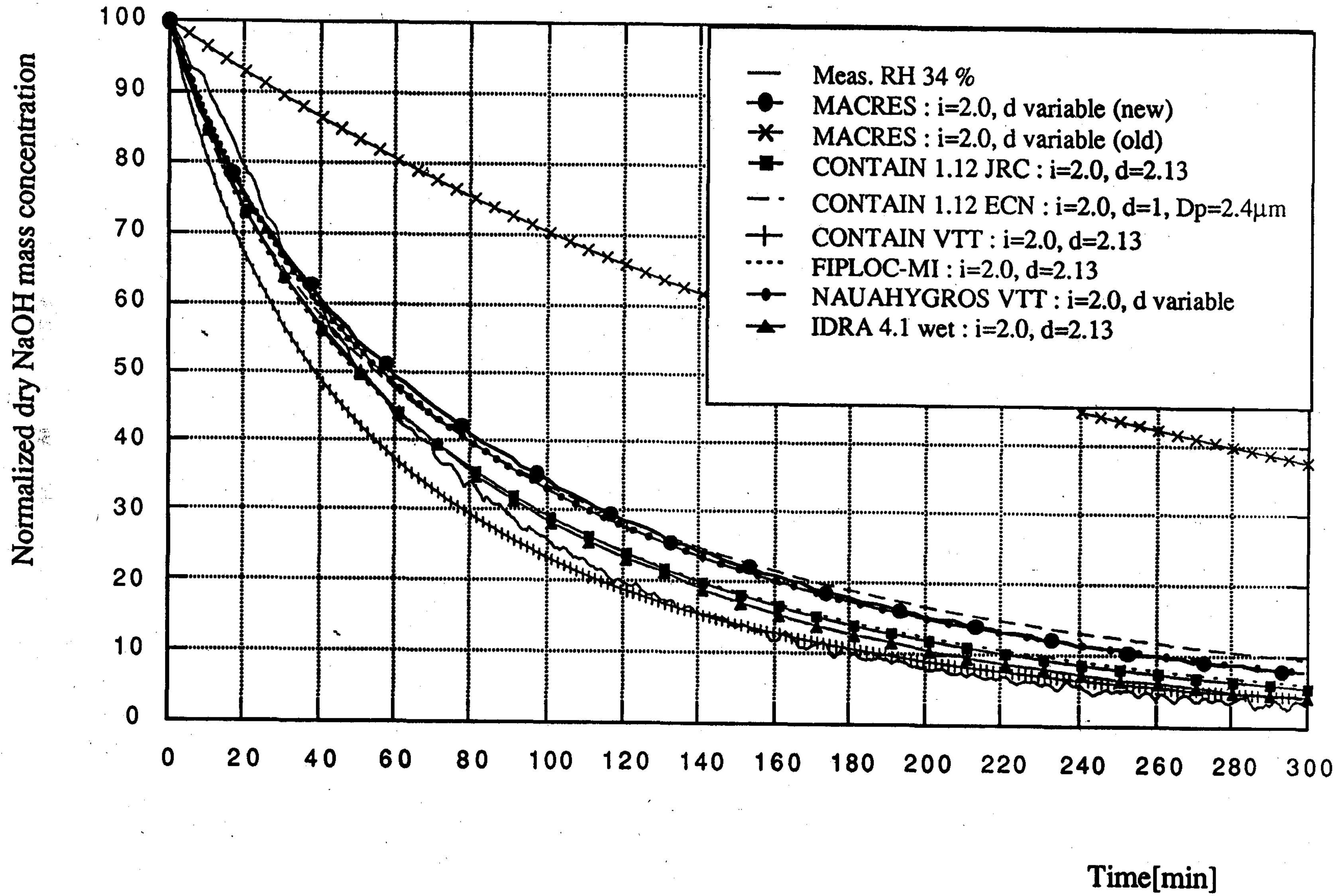
NUPEC's conclusion is that the test results are now well explained by the model of condensation on particle surface, using the original Mason's equation and applying van't Hoff coefficient 2 for ion dissociation in solution.

MACRES has performed very well in the ISP-37 (VANAM M3) Exercise, after having been revised as a result of the AHMED Code Comparison Exercise.

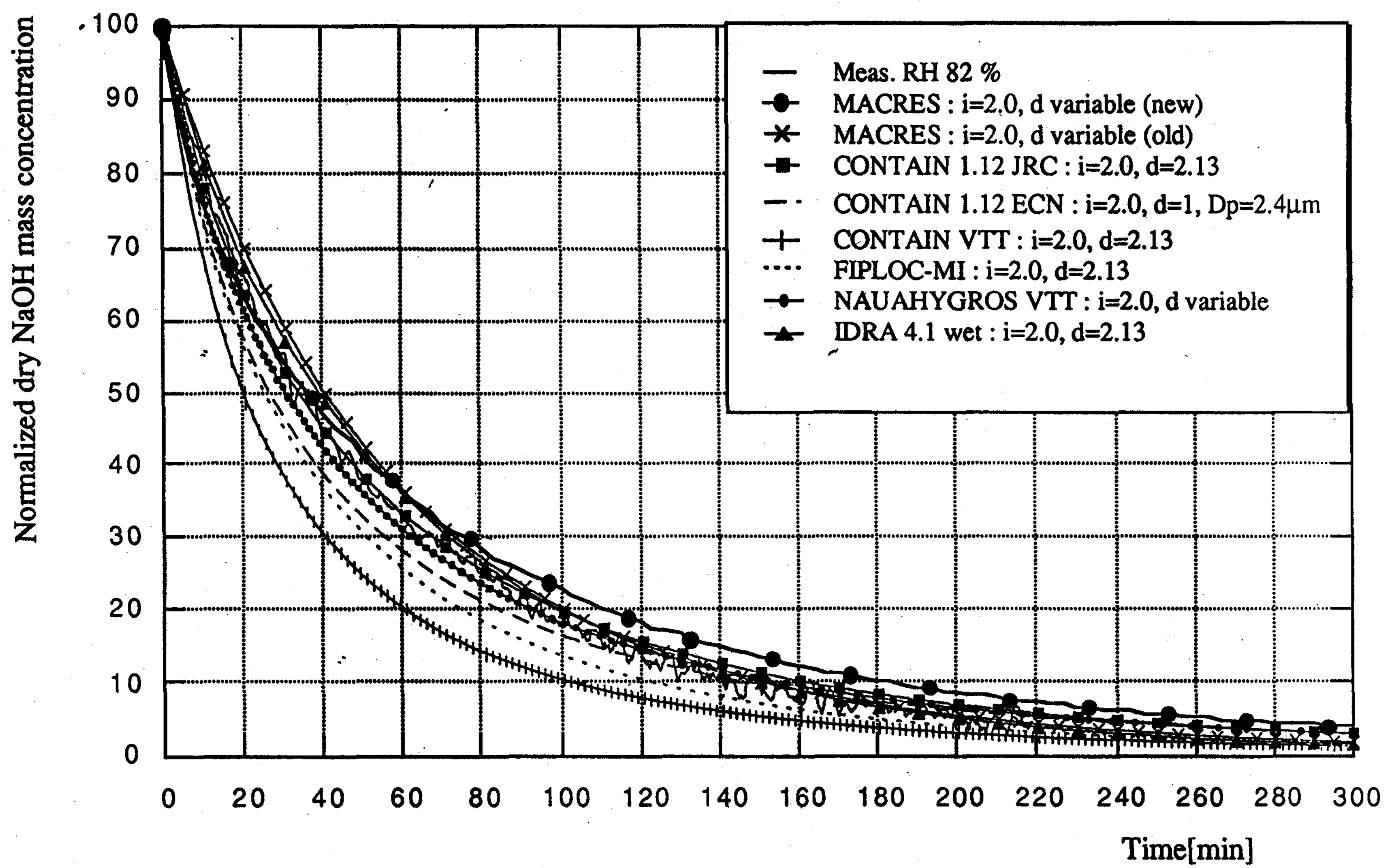
RH 22 % : Measured and calculated NaOH mass concentration time behaviour



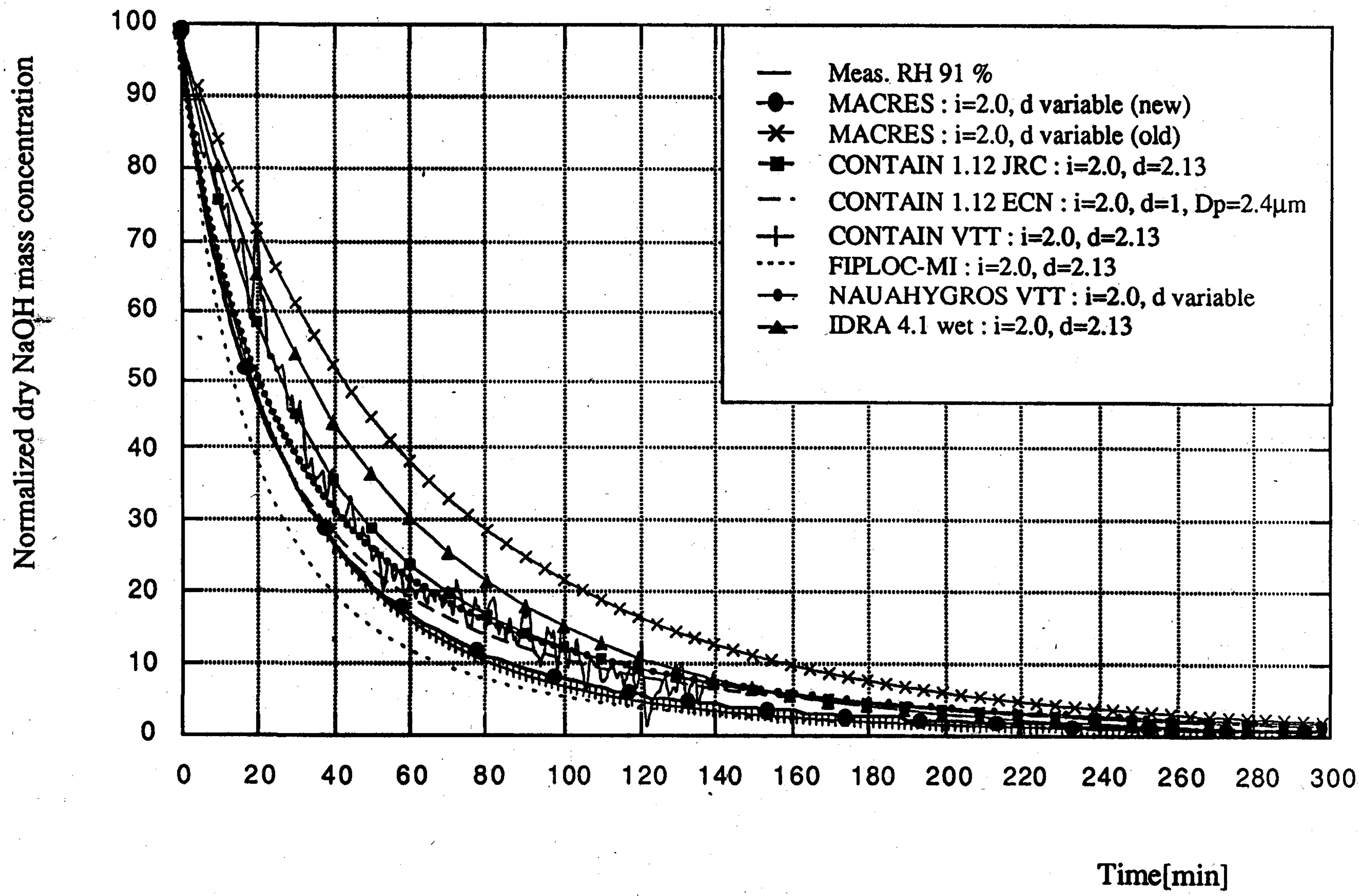
RH 34 % : Measured and calculated NaOH mass concentration time behaviour



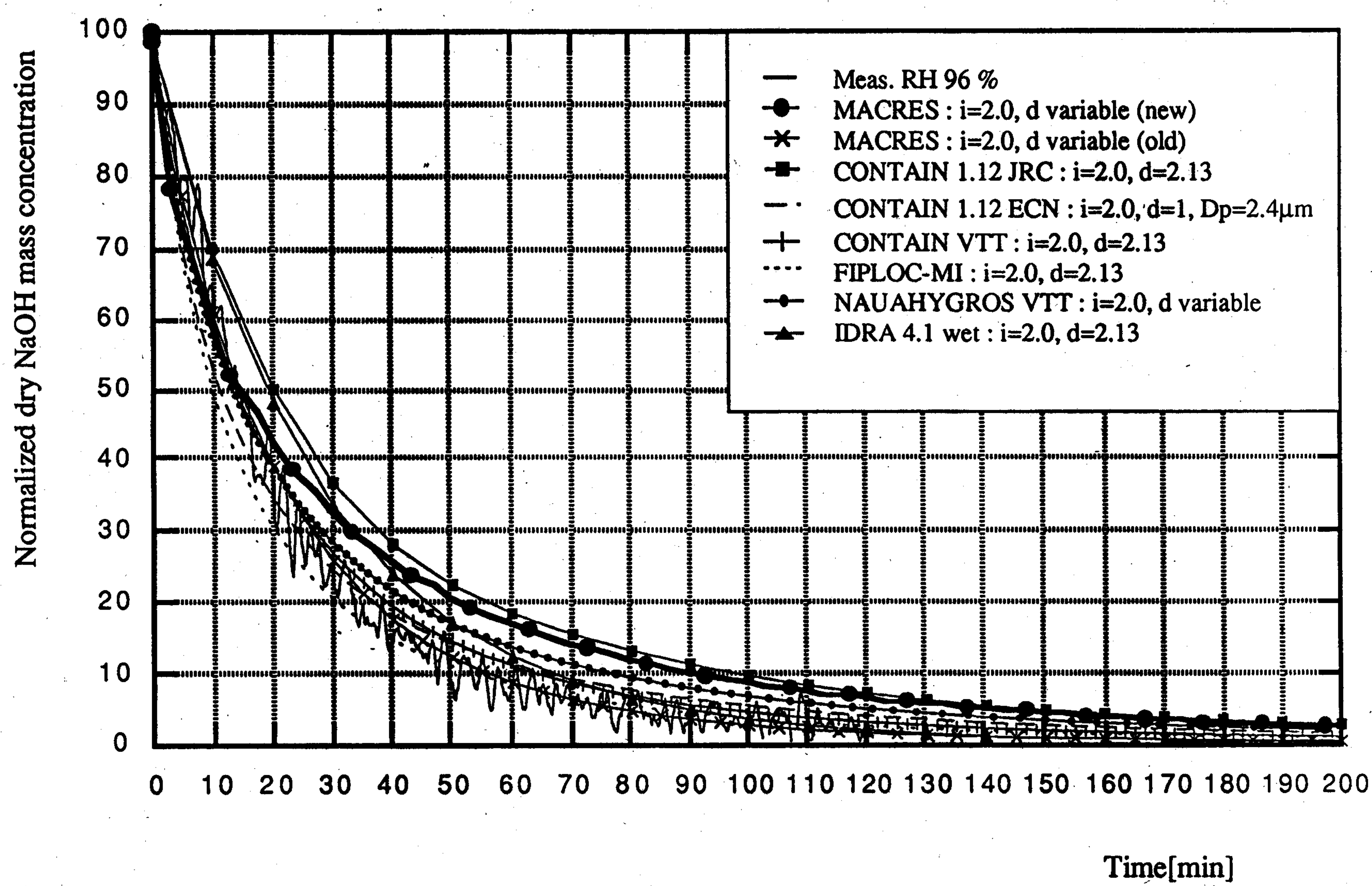
RH 82 % : Measured and calculated NaOH mass concentration time behaviour



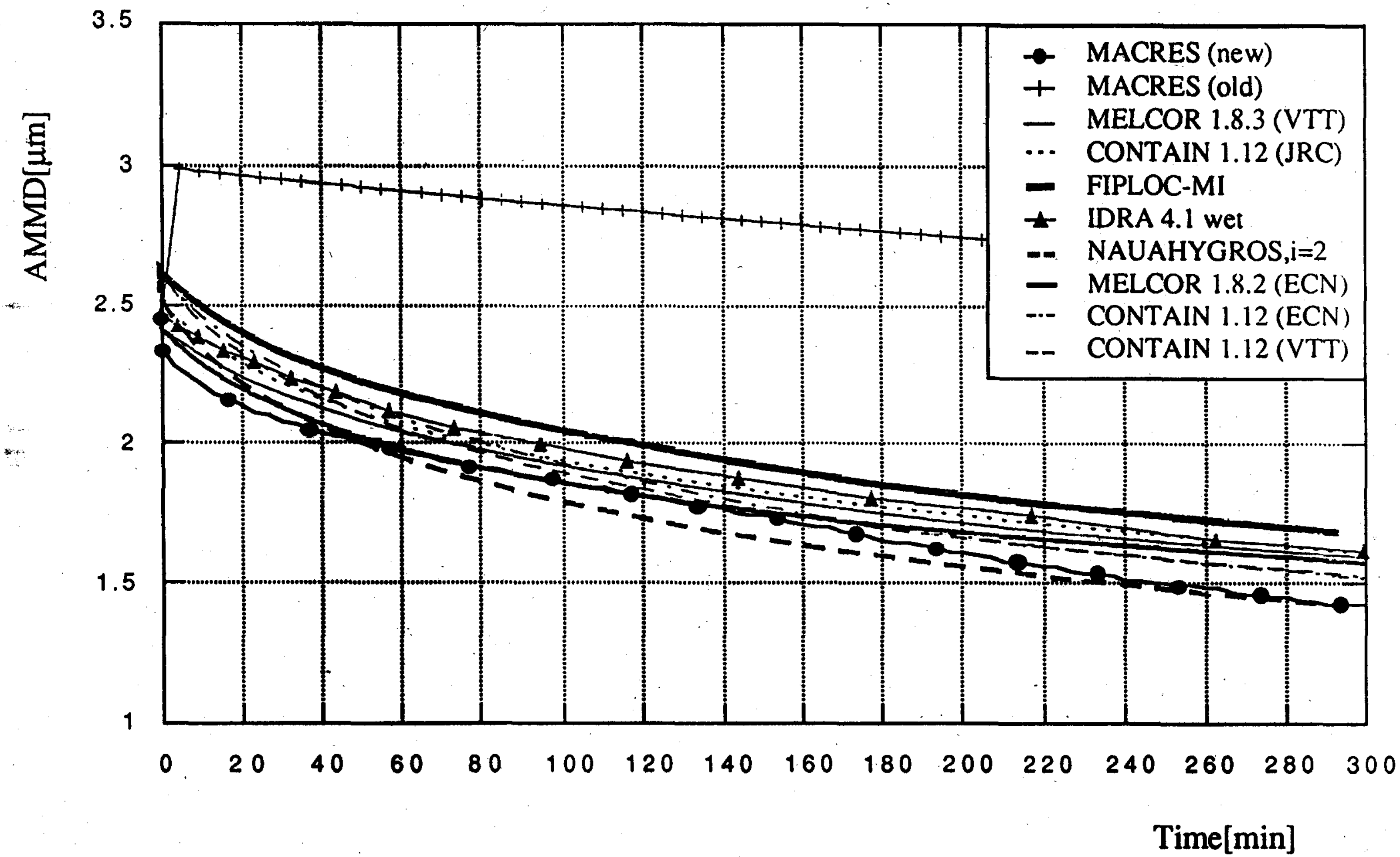
RH 91 % : Measured and calculated NaOH mass concentration time behaviour



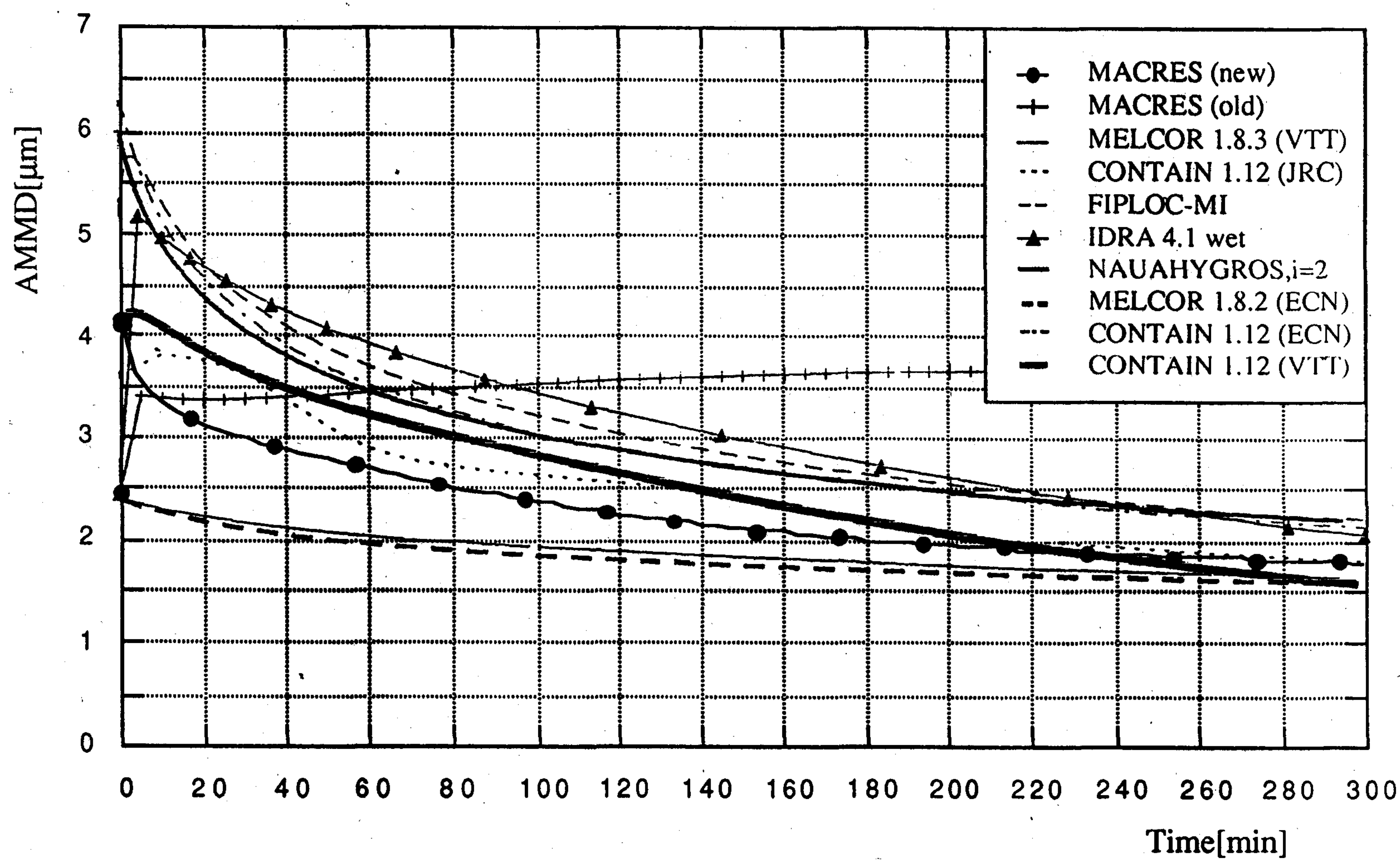
RH 96 % : Measured and calculated NaOH mass concentration time behaviour



AMMD,NaOH-test,RH 22 %



AMMD,NaOH-test,RH 96 %



AHMED CODE COMPARISON EXERCISE
REVISED DISCUSSION AND CONCLUSIONS
(prepared by J. Jokiniemi)

The codes used for the analyses of this Comparison Exercise can be divided into two groups :

1) codes including a description for the behaviour of hygroscopic particles: CONTAIN 1.12, FIPLOC-MI, NAUAHYGROS 1.1, MACRES (improved) and the second IDRA results.

2) codes which do not model the growth of hygroscopic particles: MELCOR 1.8.2, 1.8.3, and the first IDRA results.

The codes in the first group can rather well describe hygroscopic NaOH aerosol behaviour at all relative humidities. The MAEROS aerosol model used in CONTAIN and FIPLOC cannot calculate the change of particle density as NaOH absorbs water. This means that the CONTAIN and FIPLOC codes cannot correctly predict the effects of changes in particle density. However, this effect does not seem to be very dramatic at least in AHMED tests.

The MAEROS based codes CONTAIN and FIPLOC calculate the gas viscosity from dry air viscosity data. The effect of this simplification at high humidities and low temperatures, which was the case in AHMED experiments, is small. At high temperatures this effect becomes significant when the RH is high and we are in atmospheric pressure, but at higher pressures, which is usually the case in containment, the viscosity effect is not important. Thus we can conclude that the simplifications made in CONTAIN and FIPLOC to calculate the gas viscosity based on dry air viscosity do not cause noticeable errors in aerosol calculations.

The "nodal point" codes NAUAHYGROS and MACRES (improved) are able to take into account the changes in all variables during the calculation and give thus the most accurate results.

The "dry" codes MELCOR and first IDRA results belonging to the second group clearly overestimate the NaOH aerosol mass concentration being thus very conservative at high humidities.

Sensitivity calculations carried out with the NAUAHYGROS code proved that up to a RH as high as 99 % one can apply an equilibrium model, because particles reach their equilibrium size during a short time period. The equilibrium model could be one solution to decrease the conservatism of the dry codes, but still not increasing much the computing time.