NUREG-0956

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April 11, 1985

Mr. Ralph Meyer
Fuel Behavior Branch
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

Dear Ralph:

Contract No. NRC-04-84-127
Task 11

Enclosed is the long promised letter report on our TRAP-MELT/MERGE combination effort. It highlights those aspects of this effort that should be of general concern, as well as a limited selection of results from a demonstration calculation. Details of the novelties of the new code (TRAP-MELT3) relative to the TRAP-MELT/MERGE codes as used for BMI-2104 will be contained in the documentation for the code package.

There is one caveat. The figures show release fractions of core inventory up to vessel failure but do not include the source to containment resulting from suspended nuclides at the time of failure (puff release). The numbers can therefore not be readily compared to tabulated BMI-2104 values. I will send you revised figures that include this release in the near future. Since the puff release will dominate the overall release, it will reduce the difference in calculated with and without decay heat release fractions.

Submission of this report completes all efforts and satisfies the reporting requirements for Subtask 5 for Task 11, NUREG-0956 Support Calculations.

If you have any questions or comments, please give me a call.

Sincerely,

James A. Gieseke
Physico-Chemical Systems Section

JAG:drr

Enc.

cc: Sharon Wollett
Division of Contracts

REPORT

on

TRAP-MELT/MERGE MERGING

to

U.S. NUCLEAR REGULATORY COMMISSION

April 11, 1985

by

Hans Jordan

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TRAP-MELT/MERGE MERGING

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At the beginning of 1984, the U.S. NRC initiated a task at Battelle intended to investigate the effect of distributed decay heating on radionuclide transport in the primary coolant systems of LWR's during meltdown accidents. Such effects manifest themselves through a backcoupling of radionuclide transport (TRAP-MELT code) to PCS thermal hydraulics (MERGE code) and require an intimate coupling of these two (or similar) codes for their proper treatment. This task therefore consisted of a code modification and writing effort to combine the TRAP-MELT and MERGE codes and a debugging and code running effort to verify the viability of the resultant code and to illustrate, by suitable example, the consequences of including decay heating effects in the treatment of radionuclide transport.

This letter gives an overview of the modifications undertaken in TRAP-MELT and MERGE in order to combine these two codes in one code, the TRAP-MELT3 code. Included are also selected results of runs for the Surry TMLB sequence that illustrate what are expected to be the maximum consequences of the effect of decay heating on radionuclide transport during the pre-meltthrough period. In concurrence with our previous observations, based on an iterative procedure, and with the observations of others, decay heating effects appear to be of minor consequence to radionuclide transport during this period. The potentially more interesting post-meltthrough period has not yet, however, been explored, as will be explained in the following.

This letter report constitutes the conclusion of this TRAP-MELT/MERGE combination effort for the NRC.

Modifications of TRAP-MELT and MERGE and the Architecture of TRAP-MELT3

TRAP-MELT3 is a new driver routine that calls on the modified MERGE (as a subroutine) to calculate system thermal hydraulics including gas flows, gas and structure temperatures, gas pressure, gas composition, gas transport

properties, and heat transfer coefficients as averages over a MARCH time step and on the modified TRAP (as a subroutine) to calculate radionuclide transport based on these system conditions. Previously, TRAP-MELT required precalculated thermal hydraulic conditions to be read as input. These are now transmitted concurrently from the MERGE to the TRAP subroutine. In addition, previous subroutines of TRAP-MELT that were used to calculate gas properties and heat transfer coefficients could be, and have been, eliminated since these quantities are needed, and therefore calculated, in MERGE. This treatment is not only expedient, it ensures a consistency that was not achieved before. In particular, full account is taken of the steam/hydrogen mixture calculated for and control volume at each moment in time. To allow such a consistent treatment, TRAP was modified to allow for internal structures in each control volume. The primary system is therefore now nodalized in a consistent manner for both the thermal hydraulic and the nuclide transport treatment.

TRAP now tracks the fraction of core inventory of each radionuclide group that is suspended or deposited in each control volume. Deposition is further resolved by structure. This is used to calculate decay heating of gas and structures and is the only TRAP generated data used by the MERGE subroutine.

All decay energy associated with gamma rays is assumed to be absorbed by the control volume structures, i.e., no gas attenuation. The distribution of the decay heat among the structures is based on the following assumptions:

(1) Half of the energy associated with the decay heat from deposited material is assumed to be absorbed by the structure on which the material is deposited.

(2) The other half of this energy is distributed among the other structures in the control volume based upon their relative surface areas

(3) The energy associated with the decay heat from airborne material is distributed among the control volume structures, based upon their relative surface areas.

Beta decay energy is treated similarly except that allowance is taken for energy lost to the gas traversed by the beta rays. A simple model is included that approximates the amount of energy lost to the gas before impacting a structure by examining the mean range of the beta particle in the gas as a function of the gas density and particle energy.

The fraction of the beta decay energy absorbed by a control volume gas is assumed to be the ratio of the mean distance a beta particle must travel before reaching a structure (d) to the mean range of the beta particle in the gas (R). These quantities are approximated by:

$$d = \frac{4V}{A} \text{ for particles emitted from deposited radionuclides}$$

$$= \frac{2V}{A} \text{ for particles emitted from airborne radionuclides}$$

$$R = .412 \frac{1}{\rho} E_o (1.265 - .09541 \ln E_o)^*$$

where

V	=	volume of control volume
A	=	total surface area of control volume structures
R	=	mean beta particle group (cm)
ρ	=	gas density (g/cc)
E_o	=	initial beta energy (Mev).

MERGE and TRAP communicate at system time step intervals. This step is chosen to be the MARCH code time step. Over this time step MERGE iterates an internal time step that is chosen such that fractional changes in mass and energy of a control volume are limited. This internal time step also drives TRAP.

Results of a Demonstration Calculation

To illustrate the operability of TRAP-MELT3 and the effects of the superposition of decay heating on the thermal hydraulic analysis, TRAP-MELT3 was run for the Surry TMLB sequence treated in BMI-2104. Data from the MARCH code calculations for that document were used to drive the calculations. Nodalization of the primary system was however reorganized to reflect the more

*Katz, L. and Penfold, A. S., "Range-Energy Relations for Electrons and the Determination of Beta-Ray End Point Energies by Absorption", Rev. Mod. Phys., 24, 28 (1952).

rational treatment now possible in TRAP due to the inclusion of internal structures (parallel treatment of multiple structures of different thermal inertia but in the same convectively mixed gas space is now possible, for example). Thus the core region, the upper plenum, the relevant hot leg, the surge line, and the pressurizer were taken as separate control volumes. In the upper plenum, the core plate, the guide tubes (and support columns), the top plate and the annulus walls were differentiated as separate structures.

The appended figures show selected output for the comparison runs: decay heat (DH) considered; decay heat not considered (NO). The legends include the mnemonics MT (mass transfer) and FB (fall back) to indicate the use of two TRAP modifications not present for the BMI-2104 runs. These are the consideration of gas space mass transfer in the calculation of chemisorption of radionuclide vapors on surfaces and the transfer of aerosol particles from a downstream to an upstream control volume by counterflow settling (as through the core plate). The latter does not appear to have a strong influence on release to containment. The former has a pronounced effect on Te adsorption, which is now totally controlled by gas phase mass transfer.

In addition to the plot of core (grid) plate temperature as a function of time from start of melt to vessel failure (Figure 1), the cumulative fractions of core inventory of CsI, CsOH, and Te that are released to containment as a function of time are exhibited. For each species the total fractional mass as well as that attributable to the vapor and particle phases are shown.

Summary and Conclusions

Inclusion of decay heat effects in PCS modeling raises the core plate temperature by about 100 K for the Surry TMLB sequence. The core plate is the site of lowest thermal inertia and highest concentration of deposits. For other sequences the expected deposit and therefore change in temperature is expected to be less. A rise in structural surface temperature raises the vapor pressure of radionuclides deposited there and hence reduces deposition by condensation. A rise in structural temperature does not affect chemisorption rates in TRAP-MELT3 since these are taken as independent of temperature, though in general one might expect an increase in these rates. In TRAP-MELT3 only CsOH and Te are assigned a (constant) sorption rate. Under TMLB conditions

(high pressure, low diffusivity) these are sufficiently high for this mechanism to be gas phase mass transfer limited. Thus more precisely determined chemisorption rates as functions of temperature would not alter the picture significantly.

The remaining figures show a marginally higher release to containment when decay heating is considered. This is uniformly true for all three species and for all times. Note that the bulk release is in particulate form. The distribution of particle sizes released to containment is not affected. In every case the release is increased by less than a factor of two. Such a limited variation is obviously masked by larger uncertainties in the model.

Several limitations of the present approach should be mentioned. Foremost is the lack of a flow treatment past vessel failure. The problem here is that while MERGE does treat expansive flow, the direction of flow cannot now be determined mechanistically since flow resistances in the various sections of the PCS are not calculated. Ways for removing this limitation are being investigated. The question of interest here is of course the possibility of long-term reevolution of deposited radionucildes. In this vein, also, the possibility of natural convection loops through the intact legs was not considered and for the same reason. This phenomenon is of interest in that it holds promise for either additional retention or a new accident sequence!

If one calls the above limitations first order perturbations on the results, the class of second order perturbations should include aspects dealing with the extreme density of radionuclide material above the melt, such as the contribution of vapor flow to the thermal hydraulics and gas properties and the heat associated with phase changes of radionuclides. In addition, consideration must be given to the adequacy of the transport models in TRAP-MELT under these conditions.

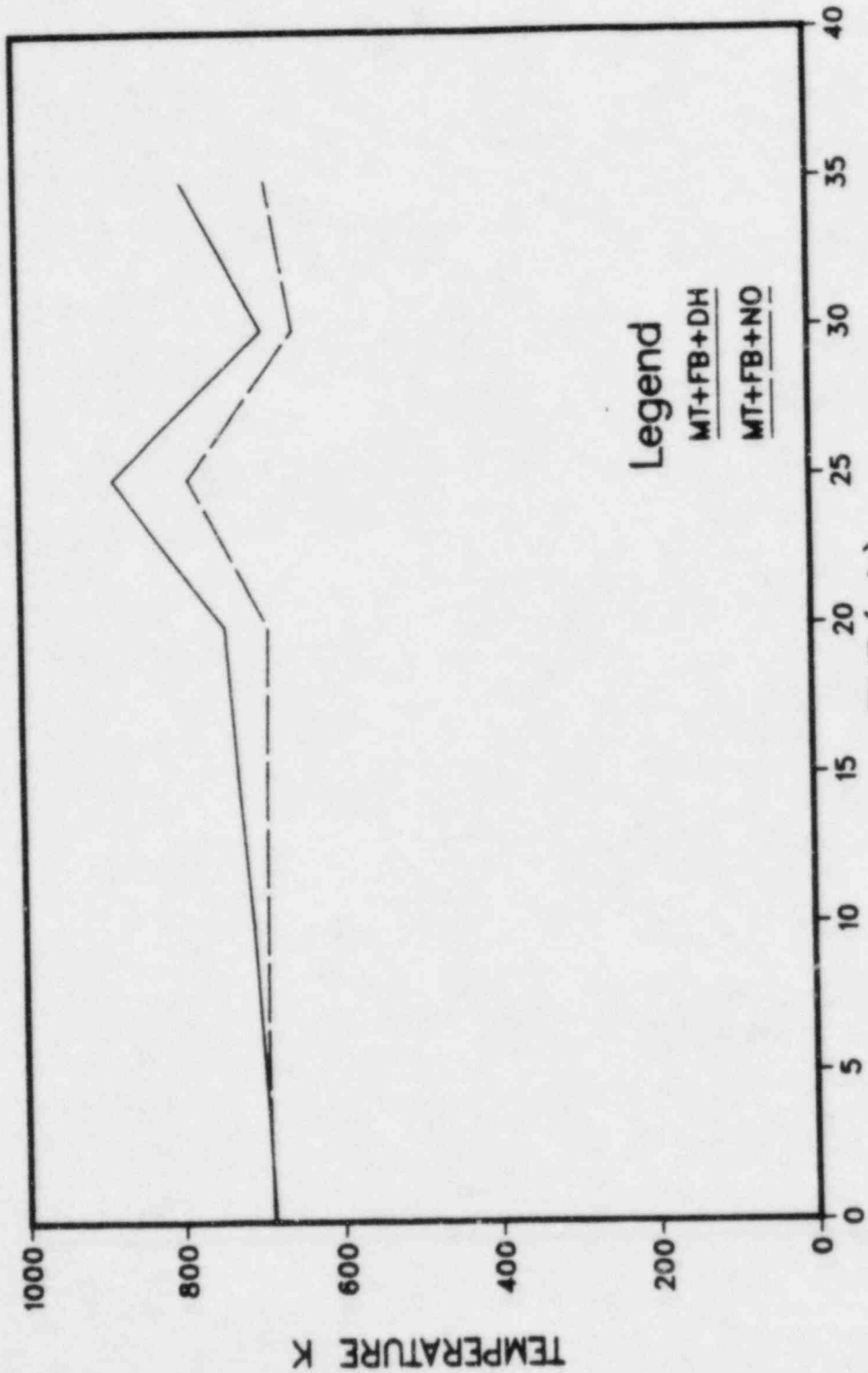

FIGURE 1. CORE (GRID) PLATE TEMPERATURE AS FUNCTION OF TIME FROM START OF MELT

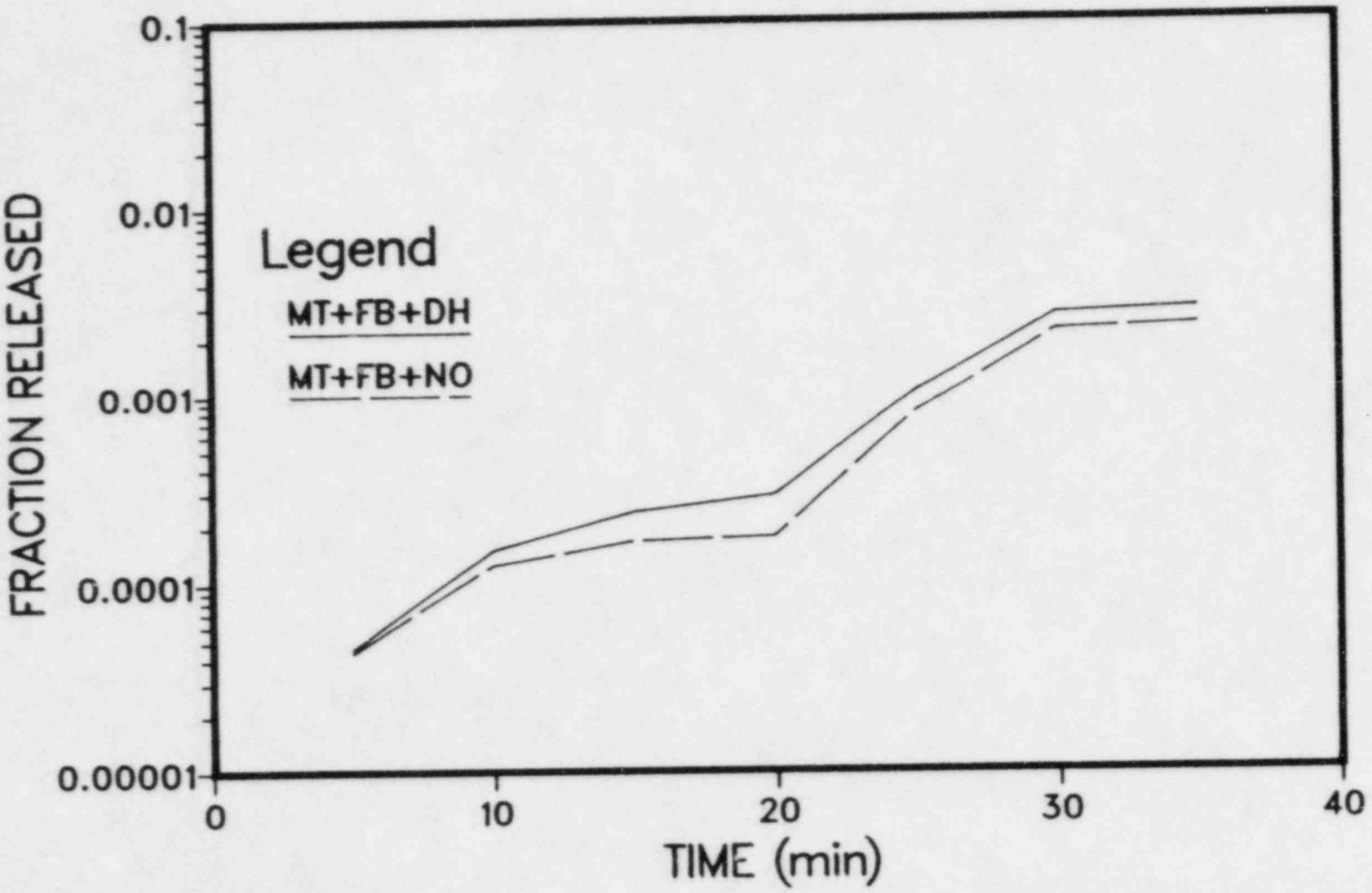

FIGURE 2. CORE INVENTORY FRACTION OF CsI RELEASED TO CONTAINMENT AS FUNCTION OF TIME FROM START OF MELT

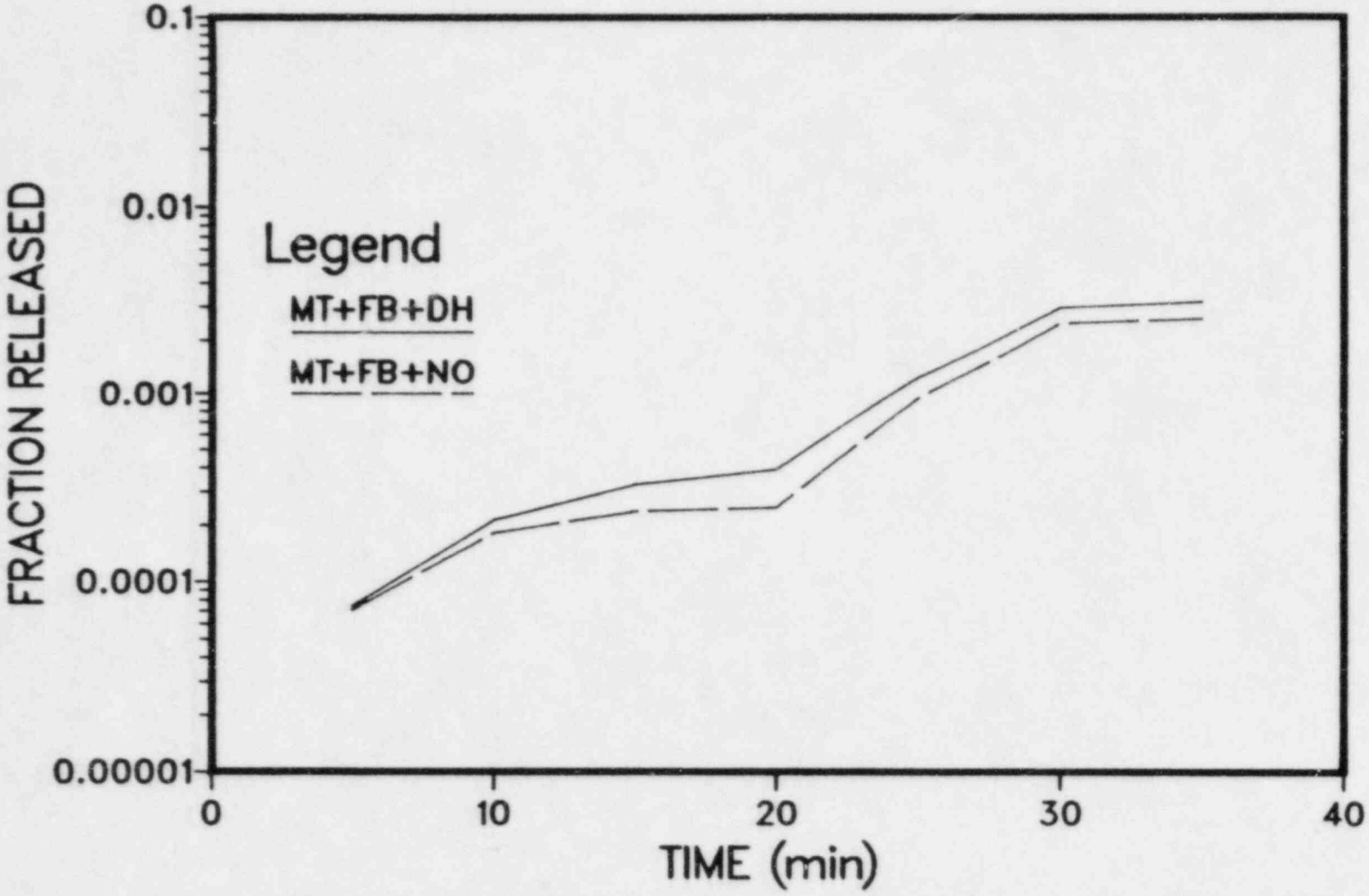

FIGURE 5. CORE INVENTORY FRACTION OF CsOH RELEASED TO CONTAINMENT AS FUNCTION OF TIME FROM START OF MELT

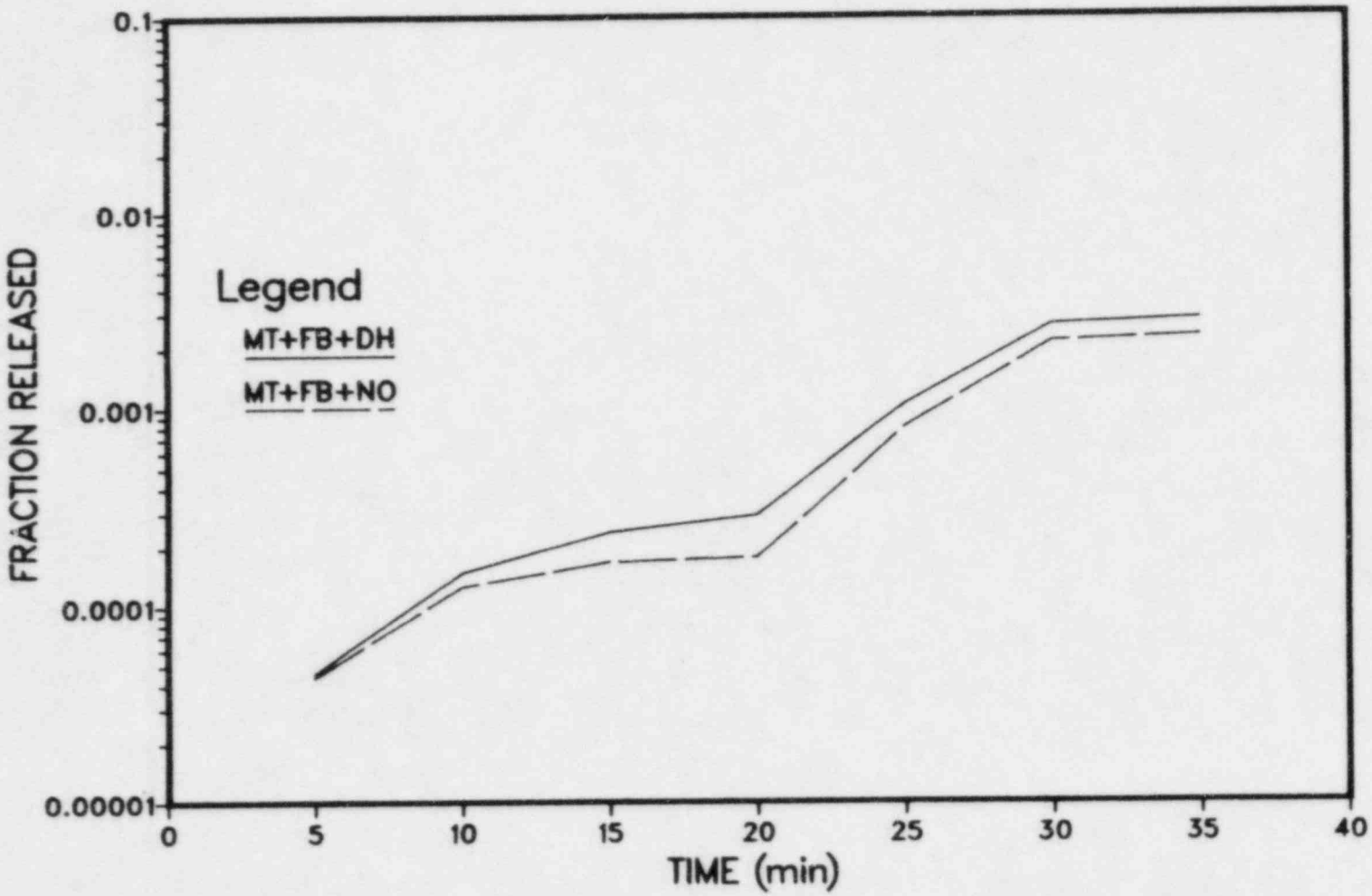

FIGURE 4. CORE INVENTORY FRACTION OF CsI RELEASED TO CONTAINMENT AS PARTICLES AS FUNCTION OF TIME FROM START OF MELT

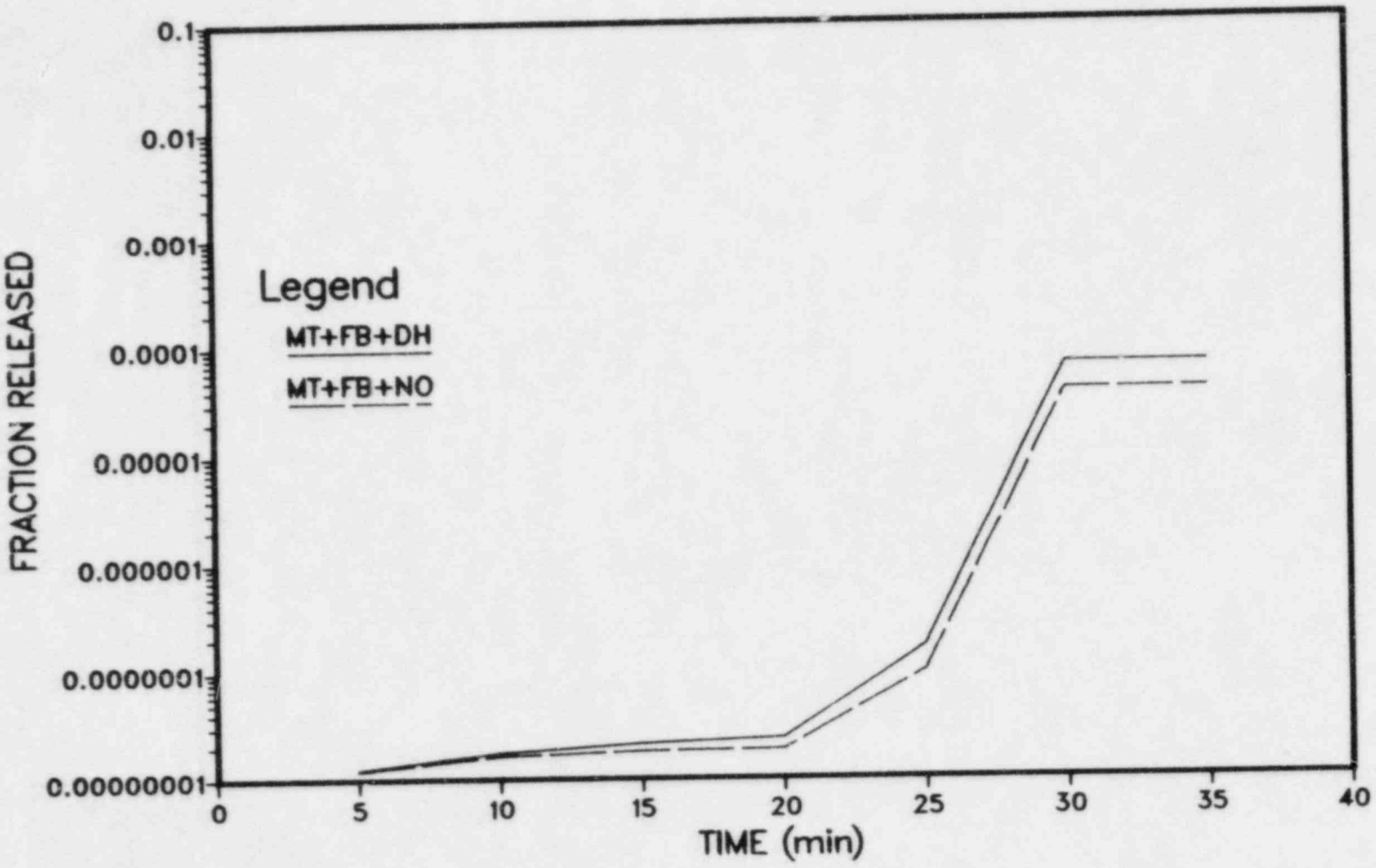

FIGURE 3. CORE INVENTORY FRACTION OF CsI RELEASED TO CONTAINMENT AS VAPOR AS FUNCTION OF TIME FROM START OF MELT

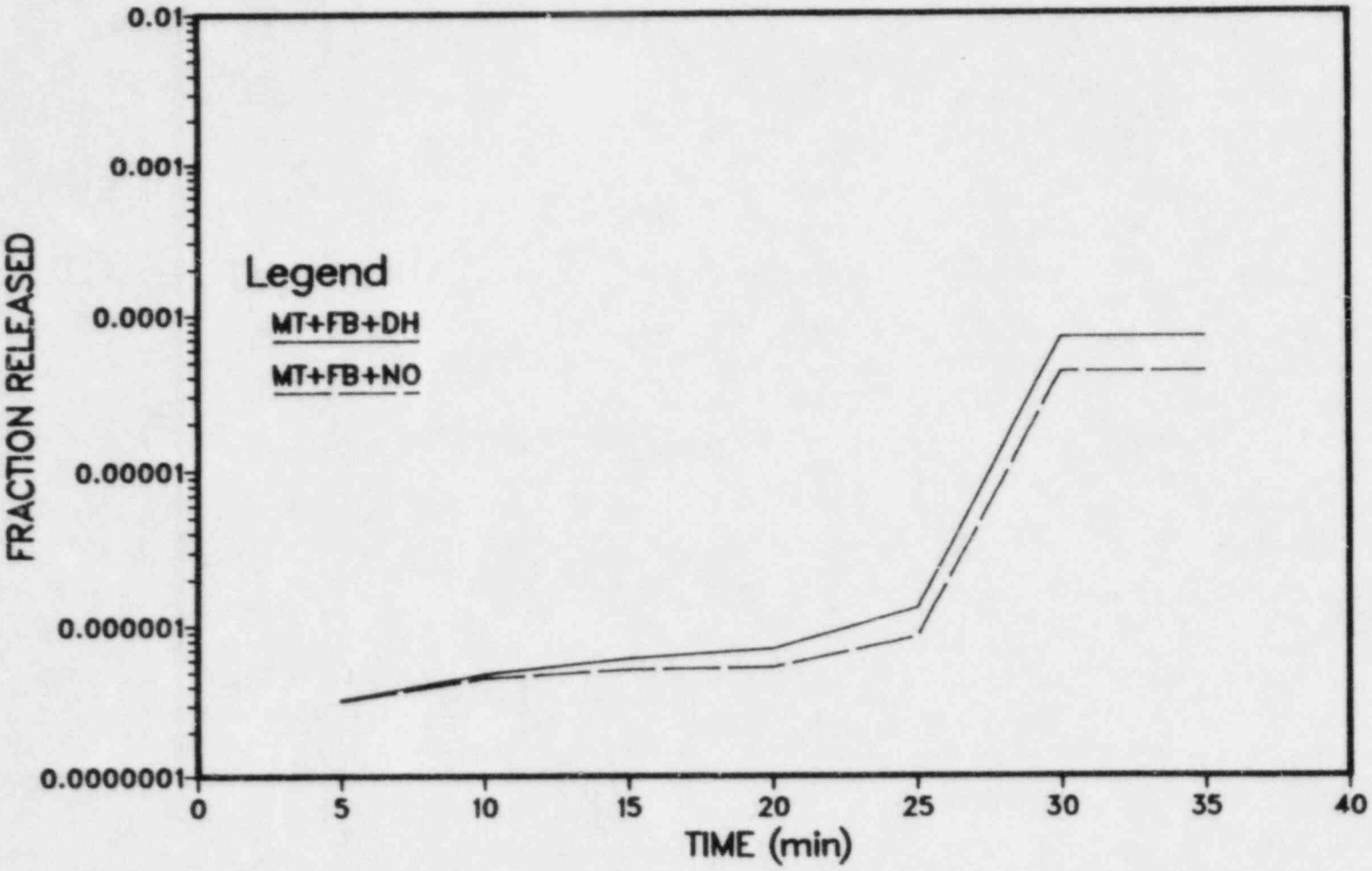

FIGURE 6. CORE INVENTORY FRACTION OF CsOH RELEASED TO CONTAINMENT AS VAPOR AS FUNCTION OF TIME FROM START OF MELT

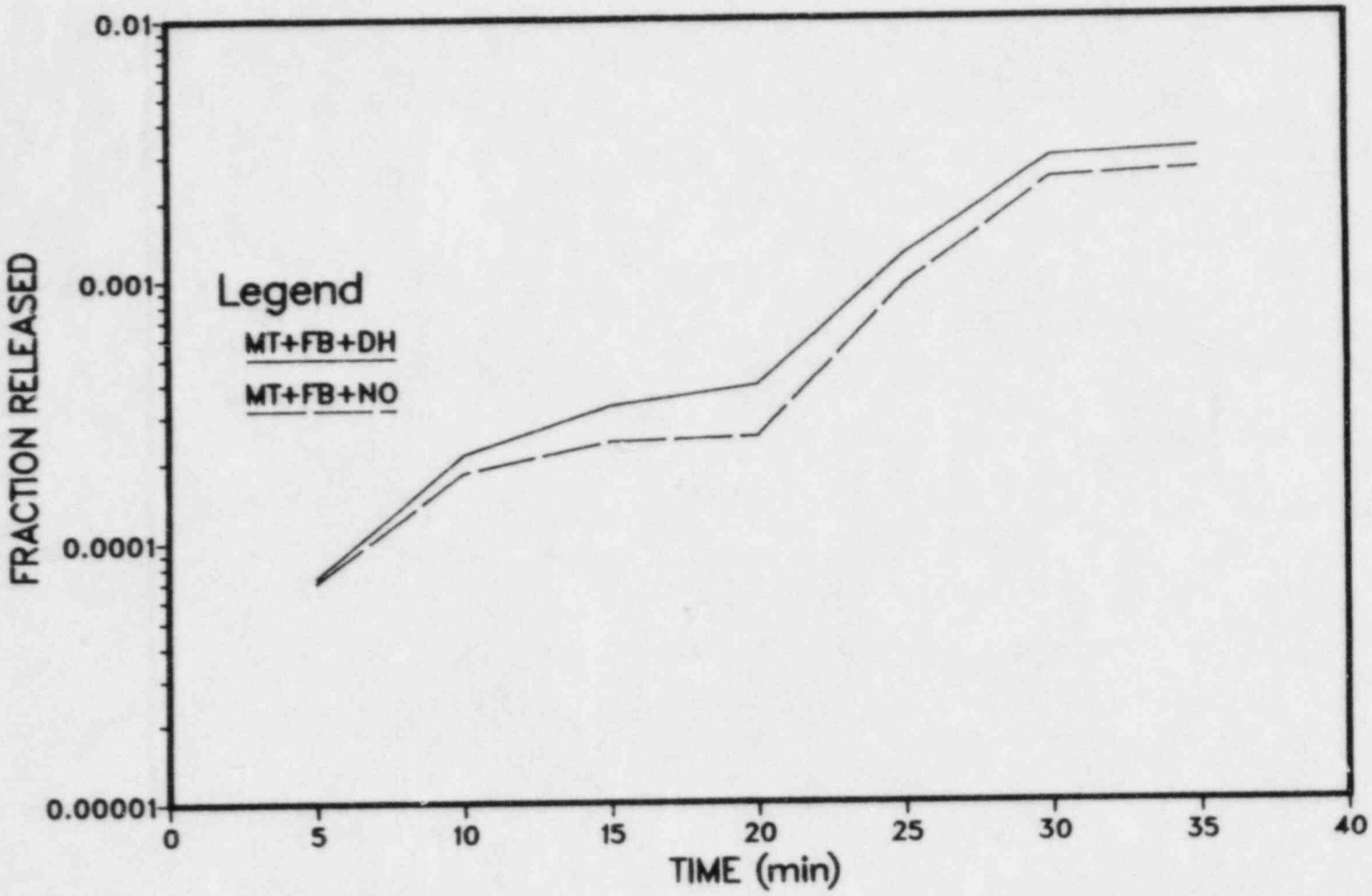

FIGURE 7. CORE INVENTORY OF CsOH RELEASED TO CONTAINMENT AS PARTICLES AS FUNCTION OF TIME FROM START OF MELT

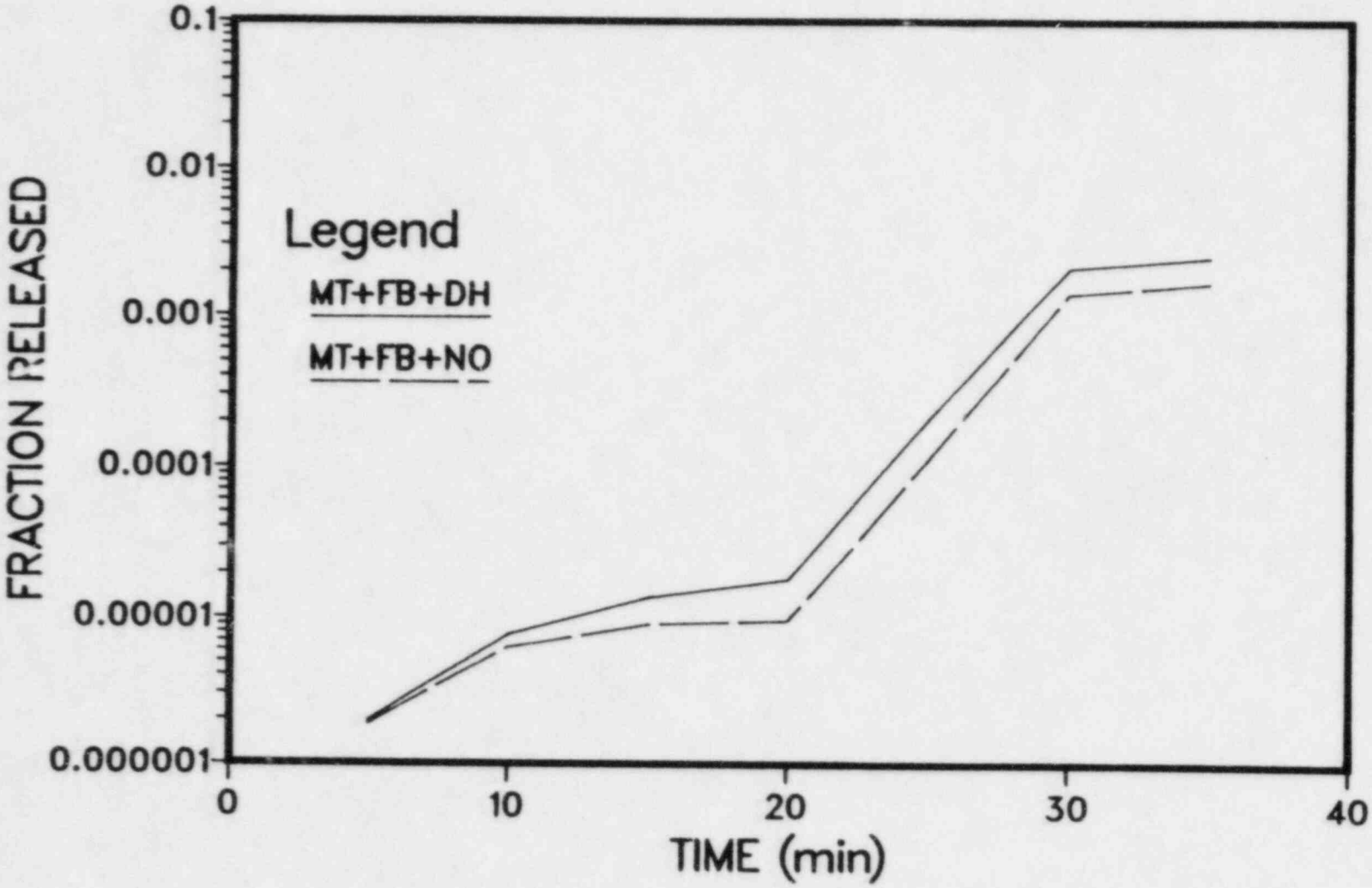

FIGURE 8. CORE INVENTORY OF Te RELEASED TO CONTAINMENT AS FUNCTION OF TIME FROM START OF MELT

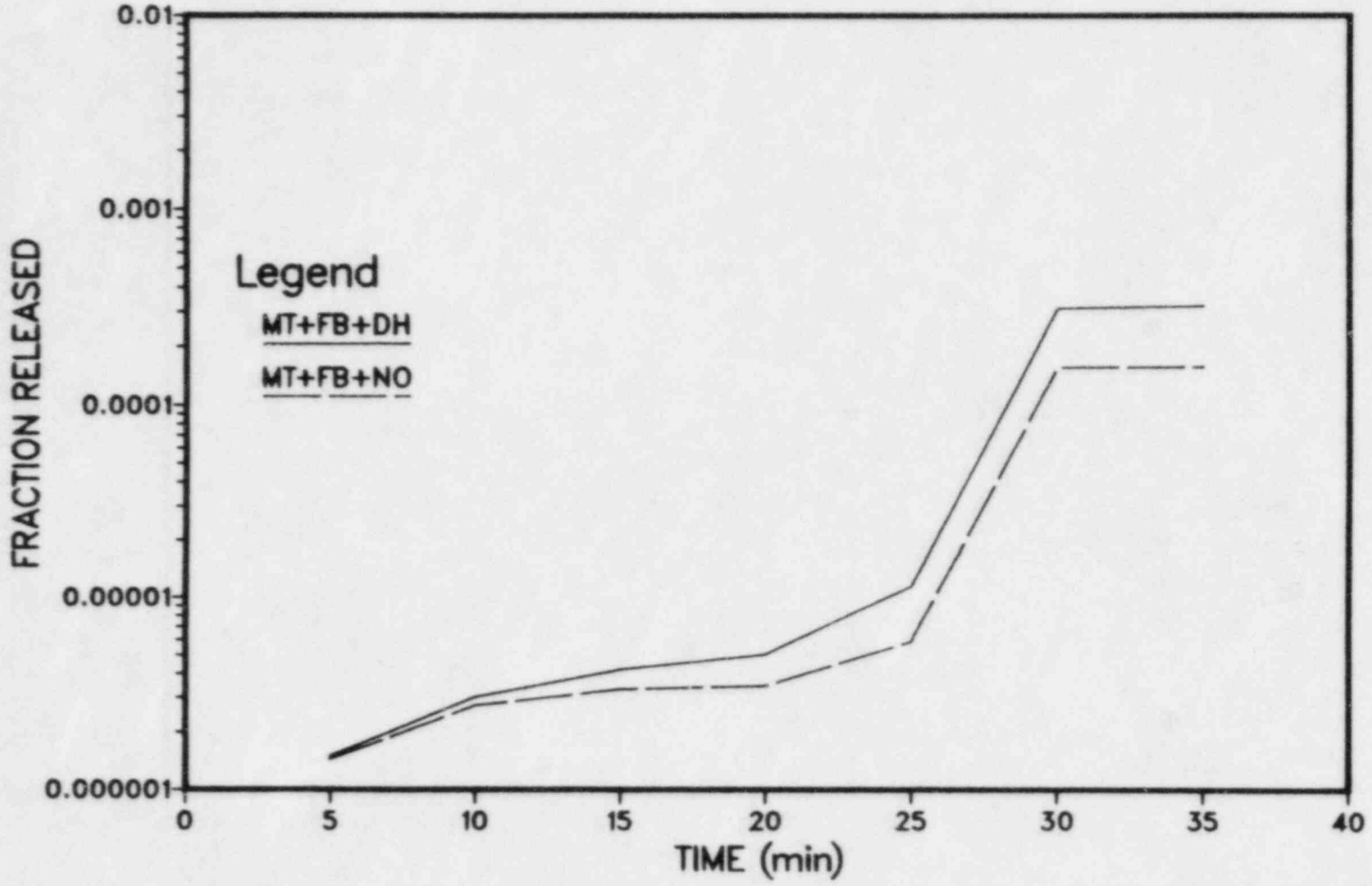

FIGURE 9. CORE INVENTORY OF Te RELEASED TO CONTAINMENT AS VAPOR AS FUNCTION OF TIME FROM START OF MELT

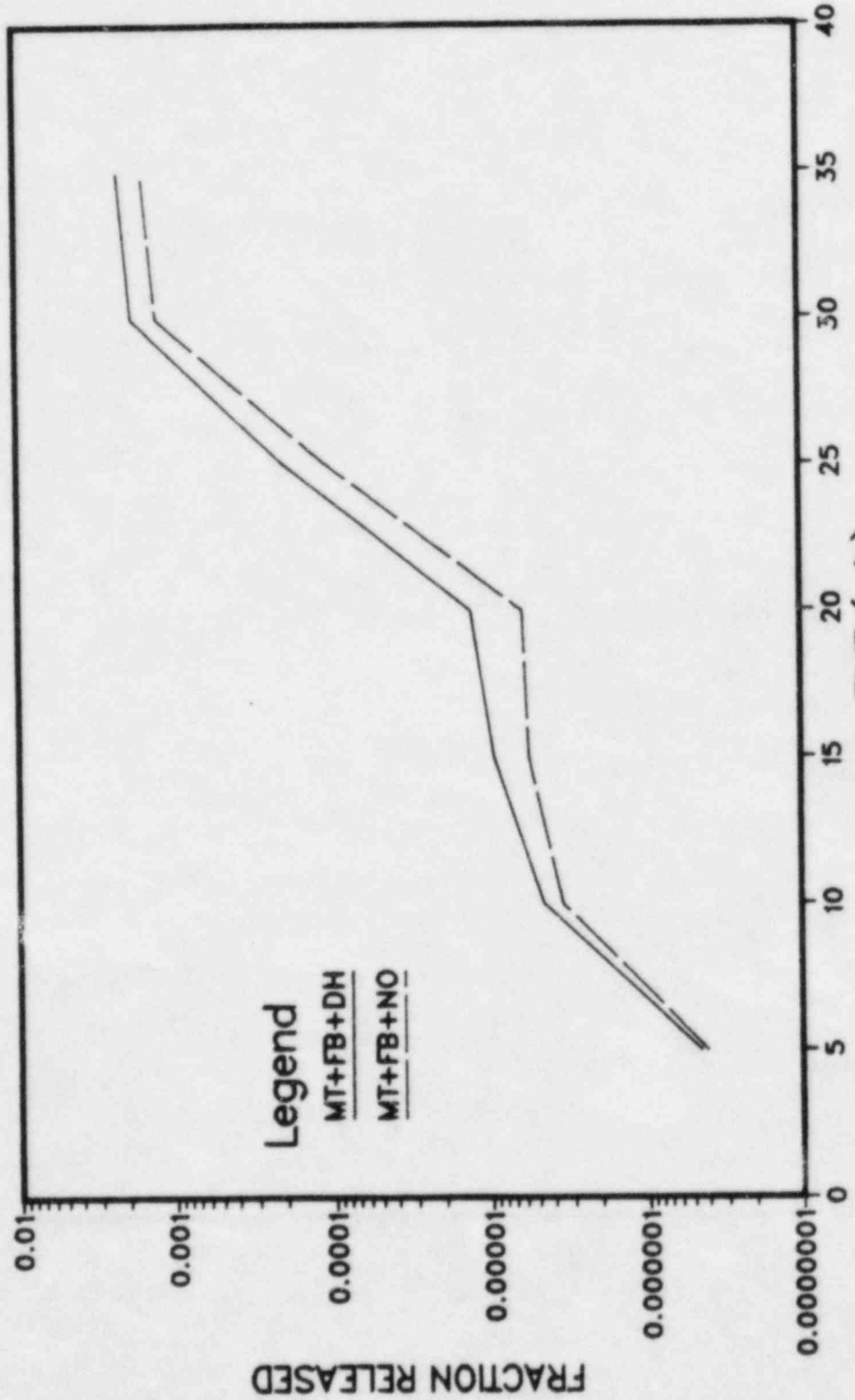

FIGURE 10. CORE INVENTORY OF Te RELEASED TO CONTAINMENT AS PARTICLES AS FUNCTION OF TIME FROM START OF MELT