Cranfield UNIVERSITY

SWATCATCH: A CATCHMENT SCALE MODEL FOR PREDICTING WEEKLY RIVER FLOWS AND PESTICIDE CONCENTRATIONS

SSLRC Report to the Environment Agency, TAPS Centre

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1.   INTRODUCTION

In March 1995, as part of the first phase of the development of a computer system for Prediction Of Pesticide Pollution In the Environment (POPPIE), SSLRC, through the project co-ordinators at the Water Research Centre, Medmenham, were commissioned by the Toxic and Persistent Substances (TAPS) Centre, National Rivers Authority, Anglian Region (now Environment Agency) to acquire and modify their existing model, SWAT, to work at the catchment level and to undertake a calibration and validation exercise on the modified model. This report gives a full description of the modified model, now called SWATCATCH, and details the results of the calibration and validation exercise.

2. MODEL DESCRIPTION

2.1 Basic Structure

The SWATCATCH model is based on the calculation of flows and pesticide concentrations contributed by each soil hydrological type within a catchment of interest. For this purpose, the catchment is divided into a number of cells as appropriate to the spatial resolution of the model input variables. For the national datasets held within POPPIE, the cells are all of 2km x 2km size. Because the model is based on a direct, empirically-derived link between soil type and stream response to rainfall (see Flow calculation, section 2.2, below), data on the exact spatial distribution of soil types within each cell is not necessary. All that is required is the fraction of each soil type within each cell and the fraction of the catchment represented by each cell. For each hydrological soil type within a cell, the Rapid runoff (Rs), Intermediate runoff (Is) and Base flow (Bs) contributions to total flow (Fs) are calculated for each timestep, along with the average pesticide concentration (CM) for each timestep and the peak pesticide concentration (CP) within the timestep. Cell values are then calculated as weighted averages based on the fraction of each soil within the cell and catchment values calculated as weighted averages based on the fraction of catchment represented by each cell. In the first version of the model, described and evaluated here, the timestep used is one week.

The SWATCATCH model has been coded in the C programming language and has been supplied to the TAPS centre through their contractors, IT Southern, as executable code with a file name of **swtctll.exe**. Detailed specifications for the model input and output file formats are set out in ANNEX I.

2.2 Calculation of Flows

The hydrological component of SWATCATCH is based upon a direct, empirically-derived link between soil type and stream response to rainfall as described in the Hydrology Of Soil Types (HOST) system (Boorman *et al*, 1995). This system groups all soils recognised in the UK into one of 29 classes based upon the hydrological characteristics of the soil and underlying substrate layer. The 29 classes have been calibrated against measured stream flow characteristics for 800 catchments across the UK (Boorman *et al* 1991). Each soil hydrological class is related to a stream flow coefficient using multiple regression based on the proportion of HOST classes in each catchment and the measured coefficient for that catchment. The two principal stream flow coefficients used are termed standard percentage runoff (SPR) and base flow index (BFI). SPR is defined as that proportion of rainfall which causes a short-term increase in streamflow over the first 24-h period after a storm event and the measured values for this parameter range from 3.8 to 77.5% for 200 catchments in the UK. BFI is that fraction of the long-term total stream volume which is represented by base flow and has measured values of approximately 0.15 to 0.95 for 575 catchments in the UK, although the soil-related coefficients have a maximum of 1.0. A third soil-related stream flow coefficient, the Intermediate Runoff fraction (IRF) has been calculated,

based on the fraction of the long-term total stream volume which is not represented by base flow and is not accounted for by SPR. IRF is calculated from:

$$IRF = (1-BFI) - (SPR/100) \tag{1}$$

If this value is negative, then IRF is set to 0.

For each soil type, Rapid runoff and Intermediate runoff are simply calculated by applying the SPR and IRF coefficients to the effective rainfall value (HER) for the timestep. Thus:

$$Rs = HER \times (SPR/100) \tag{2}$$
$$Is = HER \times IRF \tag{3}$$

However, simulations of flows in the test catchments (see section 3.1 below) showed that calculations of Rs using equation (2) slightly underestimated the measured stream response to rainfall on occasions in the summer when HER was small but total rainfall (R) was large. In such situations, rainfall-induced stream response is better simulated by using 100% of the HER as the value for rapid runoff and the model was therefore modified by transforming equation (2) as follows.

$$Rs = \textit{If } HER < 1.5 \textit{ And } R > 5, \textit{Then } HER, \textit{Else}, HER \times (SPR/100) \tag{2a}$$

Base flows (Bs) for each soil type are calculated empirically as a fraction (f_2) of a base-flow storage value (Ss).

$$Bs = Ss \times f_2 \tag{4}$$

The initial storage value (Ss^1) is defined for each soil as the product of the long term annual effective rainfall (AAHER) and the Base Flow Index, adjusted according to an empirical factor (f_1). Storage during subsequent timesteps (Ss^n) is calculated from the previous timestep storage value plus the input from effective rainfall during the timestep, minus the output from the previous timestep base flow. In this way storage, and hence base flows will gradually increase on a weekly basis during wet periods, but decrease slowly during periods with little or no effective rainfall. Thus:

$$Ss^1 = AAHER \times BFI \times f_1 \tag{5}$$
$$Ss^n = Ss^{n-1} + (HER^n \times BFI) - (Bs^{n-1}) \tag{6}$$

Where n is the number of the current timestep. The two empirical factors are directly linked according to the equation:

$$f_2 = 1 / (f_1 \times \eta) \tag{7}$$

Where η is the number of timesteps in a year. In this first version of the model the f parameters are fixed for all catchments. Calibrated values of 0.2 and 0.096 for f_1 and f_2, respectively, were calculated to give the best simulations of measured flows for the sixteen test catchments used to evaluate the model (see section 3.1, below).

Total flows (Fs) for each timestep are then calculated as the sum of the Rapid runoff, Intermediate runoff and Base flow components.

2.3 Calculation of concentrations

2.3.1 Conversion of monthly pesticide loadings to weekly loadings

The pesticide loadings datasets held within POPPIE give values on a monthly basis and these values are used as input data to the model (see ANNEX I). Because model outputs of pesticide concentrations are required on a weekly basis, a routine is incorporated within SWATCATCH that converts the monthly pesticide loading input data to weekly values. To do this, each of the 12 months is divided into 4 or 5 weeks, as appropriate to the number of days in the month. Initially, monthly loadings were then simply spread equally across all weeks in each month. However, model simulations based on this subdivision appeared to give unrealistically low predicted concentrations. It was therefore assumed that there was an uneven distribution of weekly loadings within each month. This assumption was based on the fact that the timing of most diffusely applied pesticides depends very much on local weather and soil conditions. Within a catchment, such conditions are unlikely to vary greatly and so within any month, pesticide application is likely to be concentrated during relatively short periods when conditions are favourable. Accordingly, for each month, it was assumed that half of the monthly pesticide loading was applied during a single week, one quarter during another single week and the remaining quarter distributed equally between the remaining 2 or 3 weeks. This distribution was achieved by multiplying the monthly loading value (mPL) by a fraction that represents the proportion of monthly pesticide loading assumed to be applied during a specific week. The matrix of months, week numbers and associated fractions used to convert monthly loadings to weekly loadings is as follows:

Month	Week	Conversion fraction
1	1,2	0.125
1	3	0.5
1	4	0.25
2	5,6	0.125
2	7	0.5
2	8	0.25
3	9,10,11	0.1
3	12	0.5
3	13	0.2
4	14,15	0.125
4	16	0.5
4	17	0.25
5	18,19,20	0.1
5	21	0.5
5	22	0.2
6	23,24	0.125
6	25	0.5
6	26	0.25
7	27,28	0.125
7	29	0.5
7	30	0.25

Month	Week	Conversion fraction
8	31,32	0.125
8	33	0.5
8	34	0.25
9	35,36	0.125
9	37	0.5
9	38	0.25
10	39,40,41	0.1
10	42	0.5
10	43	0.2
11	44,45	0.125
11	46	0.5
11	47	0.25
12	48,49,50	0.1
12	51	0.5
12	52	0.2

2.3.2 Peak concentrations within the timestep.

Calculation of Peak concentrations within each timestep is based on the Attenuation factor, Retardation factor and 'Minimum Standard Rainfall Volume' concepts and equations used in the simple field-scale model SWAT described by Brown & Hollis (1996). Concentrations are calculated from the concentration (C_t) of pesticide in the top 1mm layer of soil at the time of the rainfall event that causes stream response.

For each soil hydrological type a 'minimum standard rainfall volume', (MSRV) has been defined as that required to displace solute from the topsoil and impact directly on streams. No solute from the topsoil is predicted to contribute to stream response unless this amount of rainfall or more is received during a single event. When this occurs, rainfall infiltrates the soil and a proportion, equal to the MSRV is hypothesised to displace and mix with the mobile soil water fraction in the top mm of soil. This effectively dilutes the concentration of pesticide in the displaced mobile water fraction by a dilution factor, Df:

$$Df \quad = \quad Wm \, / \, MSRV \tag{8}$$

where Wm is the mobile soil water fraction in the top mm of soil which is assumed to move during leaching and is defined as the difference between the water content of the soil at 5 and 200 kPa tension (Addiscott, 1977).

The displaced mobile soil water fraction, now mixed with the minimum standard rainfall volume, is then assumed to move to surface waters, either via 'bypass' flow through the soil to drains, topsoil lateral throughflow, or overland flow. Finally, pesticide in water moving to surface waters will be subject to some sorption to soil as it moves. This is accounted for empirically by reducing concentrations of pesticide in the soil mobile water/rainfall mixture by applying a partition factor, Pf, which is independent of time and can be obtained by replacing K_{dt} with K_d in Equation (12) below.

Thus the concentration of pesticide impacting at the nearest surface water, Dc, is defined by:

$$Dc = Ct * Df * Pf. \tag{9}$$

For each timestep, the concentration (Ct) of pesticide in the top mm of soil is calculated from the total mass of pesticide (Mtm) in the top mm at the time of the minimum standard rainfall event and the volume of retained water (Wvm) in the top mm, defined as the difference between the volumetric water content of the soil at 5 kPa tension and 50% of the volumetric water content at 1500 kPa tension:

$$Ct = Mtm / Wvm \tag{10}$$

Mtm is calculated from the mass of pesticide added during the timestep (PL) and the residual mass (Mrm) of pesticide remaining from the previous timestep.

Pesticide is assumed to be added to the soil at the start of the timestep and immediately penetrate to 2mm depth. During the timestep, this added mass degrades and partitions. These processes are taken into account by applying an attenuation factor (Af_1) and a time-dependent partition factor (Pft_1) to the mass. The attenuation factor is based on soil half life and first order degradation kinetics and the time dependent partition factor is based on Koc and the equations of Walker (1987). The time used in both attenuation and time-dependent-partition-factor calculations is half the duration of the timestep (t), on the assumption that any minimum standard rainfall events always occur half way through a timestep.

$$Af_1 = EXP \{- (t/2 \times 0.693)/T_{1/2}\} \tag{11}$$

Where t is the duration of the timestep in days and $T_{1/2}$ is the pesticide half life in days.

$$Pft_1 = 1/ \{1 + (K_{dt1} \times Db) + (Ca \times Kaw) \} \tag{12}$$

Where Db is the topsoil bulk density, Ca is the topsoil drainable pore space, defined as Total pore space - water retained at 5 kPa tension, Kaw is Henrys constant for the pesticide and K_{dt1} is the time dependent sorption coefficient,.

$$K_{dt1} = K_d \{1 + (0.1 \times (t/2)^{0.5})\} \tag{13}$$

In addition to partitioning and degrading, the added pesticide mass also diffuses downwards to a specific depth, which reduces the mass in the upper mm. This is accounted for by dividing the added mass by the depth (Dp_1) penetrated during half the timestep. This depth is calculated from the topsoil hydraulic conductivity at 5 kPa tension, the duration of flow (i.e. half the timestep) and a retardation factor (Rf) for pesticide flow based on soil thin layer chromatographic theory.

$$Dp_1 = 2 + \{(t/2 \times K_{\theta5}) / Rf \tag{14}$$

$$Rf = 1 + \{(K_d \times Db) / Wi\} + \{((Ca * Kaw) / Wi)\} \tag{15}$$

where Wi is the 'retained water fraction' defined as the difference between the fraction of soil water retained at 5 kPa tension and 50% of the fraction retained at 1500 kPa tension.

Thus, halfway through the timestep (i.e. the time at which any minimum standard rainfall event is assumed to occur), the mass of pesticide remaining from that added at the start of the timestep (Mam) is calculated as:

$$Mam = (PL \times Pft_1 \times Af_1) / Dp_1 \tag{16}$$

Obviously, if no pesticide is added during the timestep, PL is 0 and thus Mam is also 0.

Pesticide residual mass (Mrm) is calculated from the total mass in the top 1mm for the previous timestep (Mtm^{n-1}) adjusted to take into account degradation, time-dependent partitioning (Pft_2) and diffusion occurring during the whole of the timestep. Degradation and partitioning are again calculated using attenuation (Af_2) and time-dependent partition (K_{dt2}) factors, but in this case based on the full duration of the timestep. Additional reduction in the residual mass resulting from diffusion taking place during the timestep is accounted for by applying a 'dilution factor' based on the ratio of the calculated depth penetrated during half the timestep (Dp_1) to the calculated depth penetrated during the full timestep (Dp_2) plus half the timestep.

$$Mrm = Mtm^{n-1} \times Pft_2 \times Af_2 \times \{Dp_1 / (Dp_1 + Dp_2)\} \tag{17}$$

Mtm for each timestep is then calculated as the sum of the Mam and Mrm.

For each soil type, peak concentrations resulting from rainfall-induced rapid runoff (Dc) are calculated only if the rainfall for the timestep is equal to or greater than the MSRV. If this is not the case, Dc is set to 0.

2.3.3 Average concentrations for the timestep.

For each soil, average pesticide concentrations (CM) are calculated from the peak concentration within the timestep (Dc) and the accumulated base flow concentration (Abc) for the timestep, adjusted to take into account the fraction of total flow (Fs) accounted for by rapid runoff (Rs), Intermediate runoff (Is) and base flow (Bs). Thus:

$$CM = [\{(Dc/2) \times Rs\} + \{(Dc/4) \times Is\} + (Abc \times Bs)] / Fs \tag{18}$$

The accumulated base flow concentration (Abc) is calculated as a running average of the base flow concentrations (Cbs) resulting from this and all previous timesteps:

$$Acb = \sum\nolimits_{n}^{1} Cbs / n \tag{19}$$

For each timestep Cbs is calculated from the mass of pesticide added (PL) and the total Attenuation factor (Aft) calculated throughout the depth of the unsaturated zone (Dz) or to bedrock, whichever is shallower. Aft is calculated from the estimated travel time (Ttl) taken by the pesticide to leach out of each significantly different layer between the soil surface and either the saturated zone, or bedrock and the pesticide half life in that layer ($T_{1/2}l$). Calculation of $T_{1/2}l$ is based on the topsoil half life ($T_{1/2}$) adjusted according to the fraction of organic carbon in the layer relative to that in the topsoil. As with the calculation of peak concentrations first order degradation kinetics are assumed.

Layer travel times (Ttl) are calculated from the layer thickness (LD-UD), the estimated average annual daily water flux (Wfs) in relation to the mobile soil water fraction (Wm) and the layer retardation factor for pesticide flow (Rfl), calculated according to equation (15).

$$Ttl = (LD-UD) \times Rfl \times (Wm / Wfs) \tag{20}$$

Wfs is calculated from the AAHER value adjusted according to the soil-related BFI to estimate average annual recharge volume (Vs) and divided by 365 to give a daily flux:

$$Wfs = (AAHER \times BFIs) / 365 \tag{21}$$

3. MODEL EVALUATION

3.1 Datasets used

Table 1. Catchments and pesticides used for model evaluation

Catchment name	Area sq. km	Characteristics	Pesticides monitored	No. of points
Wensum	557	Moderately permeable; E. Anglian chalky till over chalk	IPU MCPA	8 6
Coquet	609	Impermeable; Northern till	IPU atrazine	5 2
Hants. Stour	1235	Large	n.f.	
Idle	491	Permeable; Notts. Triassic sandstone	chlorfenvinphos endosulfan	10 31
Dove	970	Mixed; Northern till, clay, marl, Carb. sandstone & limestone	n.d.	
Worc. Stour	377	Permeable; Triassic sandstone	n.d.	
Leam	369	Impermeable; Midlands clay	n.d.	
Teifi	1006	Impermeable; Welsh hard rocks	IPU mecoprop simazine γ HCH	10 12 15 23
Darwen	142	Mixed; northern till & Carb. sandstone	atrazine simazine Chlorfenvinphos fenitrothion	14 14 14 14
Nene	210	Mixed; Jurassic limestone, ironstone & clay	IPU mecoprop methiocarb	4 4 4
Nar	227	Permeable; Norfolk chalk	IPU mecoprop methiocarb trietazine	4 4 3 2
Cuckmere	128	Mixed-; Sussex clay and Wealden loams & sandstone	simazine fenitrothion	12 12
Otter	225	Mixed; S.W. Triassic sandstone & marl with Upper Greenland	endosulfan γ HCH	7 7
Hayle	59.6	Impermeable; S.W. Hard rocks	chlorfenvinphos IPU γ HCH simazine	4 4 10 4
Severn	4330	Very large	IPU	1
Gipping	314	Moderately permeable; chalky till over chalk	n.d.	

n.f.   No relevant pesticide-specific model input files provided

n.d.   No simulations performed because of either lack of measured data, or the compounds with measured data were considered to be not diffusely applied.

In order to evaluate SWATCATCH, measured data from a total of 16 catchments representative of a range of hydrological conditions in England and Wales were provided by the UK Environment Agency TAPS Centre. The data comprised continuous weekly average flow measurements for the years 1992 to 1994 along with the individual measured pesticide concentrations from water samples taken on selected days in 1994. The characteristics of each catchment used for model evaluation are given in Table 1 along with the pesticides monitored and the number of monitoring data points.

Input parameters for the model were supplied by IT Southern and derived from ORACLE databases within the POPPIE software system. Catchment areas and the

numbers and fractions of cells within the catchment were derived as GIS functions using the Intergraph GIS within POPPIE. Pesticide physico-chemical characteristics were supplied from the PETE information system (Nicholls, 1995), and depth of the unsaturated zone was supplied by the Water Research Centre from data collected by the Environment Agency and compiled by the British Geological Survey. Spatial soil data and soil layer parameters were supplied by SSLRC from their Land Information System (Jones et al, 1993), weekly rainfall and effective rainfall were derived from the UK Meteorological Office MORECS datasets (Thompson et al, 1981) and pesticide loadings for 1994 were derived from data supplied by the Central Science Laboratory Pesticide Usage Survey group.

3.2 Hydrological evaluation

Graphical comparisons of measured and predicted flows for all 16 test catchments are given in ANNEX II, along with graphs showing the linear relationship between measured and predicted values.

Statistical comparisons of measured and predicted flows are summarised in Table 2. Addiscott & Whitmore (1987) have discussed several ways of quantifying the differences between model predictions and measured data and concluded that use of a single method might be misleading, but several methods used together could give a satisfactory summary. Accordingly, three statistical parameters are presented in Table 2. The first is simple linear regression of predicted versus measured values with the resulting equation indicating whether the model is over- or under-predicting and the overall magnitude of the error. The r^2 value indicates the consistency of over- or under-prediction. The Scaled Root Mean Square Error (SRMSE) is a measure of the spread around the ideal case where all predicted values are identical to measured values. If this is the case then SRMSE will be 0. The model efficiency is a comparison of the range of predictive errors with the range of measured values around the mean measured value. If all predicted values are identical to measured values then the model efficiency is 1. If the model efficiency is negative then the fit is unacceptably poor whereas if it is greater than about 0.5, the fit can be said to be good. Both these parameters have been used in a comprehensive evaluation of the performance of pesticide leaching models (Walker et al, 1995).

The overall statistics based on measured and predicted values for all catchments suggest that, across the wide range of measured flows, the model is giving a very acceptable fit. The linear regression equation shows that, nationally, there is no general tendency for either over- or under-prediction of flows.

Individual catchment statistics given in Table 2 show that, in general, with the exception of the Hayle and the Otter, the smaller the catchment, the poorer the flow estimation. This undoubtedly reflects the base resolution of the data used to derive model input parameters. In particular, the coarse resolution of MORECS data could lead to predictive errors in small catchments, because flow predictions are likely to be most sensitive to significant variations in HER. Nevertheless, for all but 2 of the test catchments the SRMSE is less than 1, whereas the model efficiency is unacceptably poor (a -ve value) for only 3 catchments but good (> 0.5) for 7 catchments.

Table 2. Statistical comparisons of measured and predictive flows for the representative catchments

Catchment Name	Area sq. km	Characteristics	Meas. vs. pred linear regression R squared	Equation	Scaled RMSE	Model Efficiency
Hayle	59.6	Impermeable	0.604	y = 0.6956x + 0.3598	0.521	0.591
Cuckmere	128	Mixed	0.4181	y = 0.7053x + 0.4856	1.294	0.183
Darwen	142	Impermeable	0.6495	y = 0.4776x + 0.6435	0.6535	0.4193
Nene	210	Mixed	0.5313	y = 1.131x - 0.2575	0.751	-0.161
Otter	225	Mixed	0.6618	y = 0.7883x + 0.589	0.603	0.637
Nar	227	Permeable	0.8543	y = 2.4121x - 0.5831	1.4152	-3.8339
Gipping	314	Moderately permeable	0.7709	y = 1.207x + 0.0351	0.842	0.484
Leam	369	Impermeable	0.6246	y = 0.7778x + 0.3258	0.8316	0.5841
Worc. Stour	377	Permeable	0.498	y = 1.2051x - 0.2059	0.583	-0.584
Idle	491	Permeable	0.7235	y = 1.3319x - 1.0571	0.536	0.1711
Wensum	557	Moderately permeable	0.8719	y = 1.4839x - 0.9653	0.655	0.342
Coquet	609	Impermeable	0.634	y = 0.5935x + 1.1593	0.799	0.571
Dove	970	Impermeable	0.6123	y = 0.5097x + 1.0662	0.661	0.3326
Teifi	1006	Impermeable	0.7459	y = 0.6992x + 9.8808	0.4375	0.743
Hants. Stour	1235	Large	0.6116	y = 0.6482x + 4.0118	0.634	0.607
Severn	4330	Very Large	0.8247	y = 0.9227x + 18.302	0.4512	0.7596
All catchments			0.8733	Y = 0.9999X + 0.3145	0.8952	0.8548

Examination of the linear regression equations shows that for 'impermeable' catchments the model always underpredicts flows, whereas for 'permeable' catchments the model consistently overpredicts flows. This is almost certainly the result of using a single set of 'average' values for the empirical factors used to calculate the base flow component of total flow (see section 2.2). The implication is that future developments of the model could give improved predictions of flows by using different base flow factors, depending on the general catchment hydrogeological characteristics.

Of the three catchments with an unacceptably poor model efficiency, the R. Nar is by far the worst case. It also has the highest SRMSE. Examination of the graphical comparisons for this catchment, given in ANNEX II, shows a very large discrepancy between measured and predicted flows with the model consistently overpredicting flows by a factor of almost 2.5 (r^2 of 0.8543). The Nar catchment is dominated by chalk and chalk-derived soils and the measured flows show a pattern dominated by base flow with a very muted response to rainfall, particularly in the winter of 1992. This contrasts strongly with predicted flows which show significant responses to rainfall. In the adjacent Wensum catchment, dominated by chalky till over chalk, model simulations have the next highest over-prediction factor (1.48) although the ME and SRMSE are much better (0.342 and 0.655 respectively). In this case, model over-prediction appears to result mainly from overestimation of the rapid and intermediate runoff components of flow, as the base flow levels look to be well matched. This pattern is repeated in the other E. Anglian test catchment, the Gipping, also dominated by chalky till over chalk.

Clearly, in E. Anglia, the model is overpredicting the runoff components of flows, whereas in the pure chalk catchment of the Nar, it also appears to drastically overpredict the base flow component during the autumn, winter and early spring periods. The exact reasons for this are not clear, but most likely relate to the hydrogeological characteristics of both the chalk and chalky tills in the area, which may be significantly misrepresented by the model. Alternatively, they could relate either to an overestimation of HER using MORECS, in this, one of the driest parts of the

country, or to a poor spatial representation of the soil pattern on the 1 : 250,000 scale base maps used to derive the spatial soil datasets.

After the Nar, the catchment with the next worse model efficiency is the Worcestershire Stour. However, in this case the evaluation statistics are less clear. They suggest that, whereas on average the model predictions are relatively good with small errors (SRMSE has one of the lowest values and the over-prediction factor represented by the regression equation is one of the smallest at 1.2), the predictions are inconsistent and the overall 'fit' of the measured and predicted hydrographs is poor. This possibly results from a combination of a relatively small catchment with a significant urban component and a flow gauging station located well upstream from the catchment outlet used to generate model input data.

The final catchment with an unacceptably poor ME is the R. Nene. For this catchment, the SRMSE is towards the higher end of the range and, although the regression equation shows a relatively small over-prediction by a factor of 1.13, the predictions are inconsistent, with an r^2 of only 0.53. The Nene catchment is relatively small, with a classic mixed hydrogeology comprising complex, interbedded, strongly contrasting impermeable clays and permeable limestones and ironstones, all of Jurassic age. In these formations, there is significant local variation in the relationships between clay and limestone or ironstone beds and this can significantly affect stream response to rainfall. Because of this complexity, the national scale of the spatial soil parameter datasets used in POPPIE may significantly misrepresent local soil patterns and the nationally-derived empirical soil-related stream flow coefficients may be very unrepresentative for small areas. Both these factors could have resulted in the poor model predictions and are likely to give similar problems when using the model in other relatively small catchments with similar complex Jurassic lithologies.

For the test catchments of the Idle, Darwen, Wensum, Dove, Gipping and Cuckmere, model efficiencies are acceptable, but less than good. Possible reasons for the less than good fits in the Wensum and Gipping have been discussed above. For the Idle catchment, although the model efficiency statistic is low, the SRMSE is also among the lowest, at 0.536. As with the Worcestershire Stour, these are somewhat conflicting evaluation statistics. Examination of the graphical comparisons in ANNEX II shows that the measured hydrograph for the Idle has some curious 'level' base values and it is possible that these represent either problems with the gauging equipment or some artificial influence on the river. Resolution of these discrepancies will therefore require further investigation. The Darwen, Dove and Cuckmere are all catchments with 'mixed' impermeable and permeable or moderately permeable hydrogeologies. In addition, the Darwen has a significant urban component and the Cuckmere is one of the smallest catchments tested. All these factors are likely to contribute to their less than good model efficiency statistics.

3.3   Evaluation of Pesticide concentrations

Graphical comparisons of the selected catchments and pesticides detailed in Table 1 are given in ANNEX III. Because of the limited measured data available, it is very difficult to undertake any meaningful evaluation of the SWATCATCH model with respect to its simulation of pesticide concentrations. However broad comparisons of the predicted ranges with the measured ranges and detection levels for all the pesticides studied are given in Table 3. The comparisons suggest that, with the exception of γ HCH, atrazine, chlorfenvinphos, endosulfan in the Idle catchment and simazine in the Hayle catchment, model predictions are very acceptable. For those weeks with measured data, all predictions are within one order of magnitude of positive detections and, in most cases, are below the level of detection concentration when measurements indicate they should be so. In addition, for those situations where predicted concentrations are less than one third of their equivalent measured values (IPU & MCPA in the Wensum, mecoprop in the Teifi and simazine in the Cuckmere), the maximum predicted concentration within all weeks of the simulation is always either more than or between one half and one third of the measured value.

The poor predictions for γ HCH, atrazine and chlorfenvinphos are not surprising. γ HCH is widely used in agriculture, but also has a significant non-agricultural usage, both as a wood and a medical treatment. The main agricultural usage of chlorfenvinphos is in sheep-dip. As such, the presence of both compounds in surface waters is not likely to be related to diffuse agricultural usage. Similarly, the main use of atrazine, prior to 1994, was non-agricultural and gave rise to significant residues in many water resources. Although its non-agricultural usage was banned in 1994, its physico-chemical characteristics suggest that environmental residues from non-agricultural usage are likely to persist for some time and could be giving rise to the significant measured residues, particularly in the Darwen catchment which has a relatively large urban component.

Reasons for the unsatisfactory predictions of endosulfan residues in the Idle catchment and simazine residues in the Hayle catchment are less obvious. Within the Idle, endosulfan has been detected at concentrations of 11 to 12 ng/l, whereas simulation suggests that values should not exceed 0.04 ng/l at any time during the year. However, of the 31 measurements of endosulfan within this catchment, only 2 had positive detections, although both occurred at the time when simulations suggested that the compound was appearing in surface waters. It is possible therefore, that the large difference between measured and simulated concentrations could result either from 'point-source' pollution associated with agricultural usage, or from the way in which the model distributes the monthly pesticide loadings across the 4 or 5 weeks of each representative month. Model simulation errors related to the latter possibility are discussed in more detail in the paragraphs below.

Within the Hayle catchment, simazine was measured on 4 occasions but was always below the detection level of 5 ng/l. In contrast, model simulations predict that, throughout the year, concentrations will always be between 42 and 153 ng/l. This is in strong contrast to all other catchment simulations, where there is a very consistent

Table 3. Summary data for measured and predicted pesticide concentrations (ng/l)

Catchment	Pesticide	Detection level	Number of measurements	Number not detected	Measured range	Predicted range for weeks with measured data	Predicted range for all weeks
Wensum	IPU	20	8	1	30 - 720	58 - 177	14 - 413
	MCPA	20	6	5	39	2 - 6	1.3 - 197
Coquet	atrazine	5	2	0	5 - 6	0.04 - 0.3	0.03 - 0.3
	IPU	20	5	2	80 - 140	6 - 70	1.6 - 130
Idle	chlorfenvin.	10	10	9	18	0.13 - 0.28	0.08 - 0.28
	endosulfan	5	31	29	11 - 12	0 - 0.04	0 - 0.04
Teifi	IPU	100	10	10	n.d.	2 - 6	0.8 - 24
	γ HCH	5	23	23	n.d.	0	0
	mecoprop	100	12	9	140	0.7 - 10.8	0.5 - 69
	simazine	10	15	15	n.d.	1.2 - 4.1	0.7 - 8.3
Darwen	atrazine	5	14	10	41 - 101	0.2 - 1.3	0.2 - 8.4
	chlorfenvin:	10	14	13	170	0.03 - 0.12	0.02 - 0.12
	fenitrothion	10	14	14	n.d.	0 - 0.03	0 - 0.16
	simazine	5	14	12	17 - 113	1.6 - 5.3	1.0 - 6.2
Nene	IPU	20	4	0	30 - 210 (34800)*	14 - 482	3 - 1280
	mecoprop	40	4	1	24 - 363	0.1 - 312	0.1 - 384
	methiocarb	10	4	4	n.d.	0.5 - 2.2	0 - 5.4
Nar	IPU	20	4	2	60 - 220	69 - 101	32 - 260
	mecoprop	40	4	2	23 - 39	1 - 36.6	0.5 - 325
	methiocarb	20	3	3	n.d.	0.06 - 0.1	0.05 - 5.7
	trietazine	20	2	2	n.d.	1.6 - 1.7	0.8 - 2.0
Cuckmere	simazine	20	12	7	20 - 89	7 - 26	3.8 - 38
	fenitrothion	20	12	12	n.d.	0 - 0.2	0 - 0.2
Otter	endosulfan	6	7	7	n.d.	0 - 0.01	0 - 0.04
	γ HCH	4 - 20	7	6	18	0	0
Hayle	chlorfenvin.	18 - 19	4	3	92	5.1 - 10.4	2.8 - 10.7
	IPU	40	4	4	n.d.	6 - 12	4.4 - 44
	γ HCH	3.3 - 5	10	9	6.3	0	0
	simazine	5	4	4	n.d.	54 - 153	42 - 153
Severn	IPU	100	1	1	n.d.	38	16 - 359

* Very large value likely to be the result of point source pollution or analytical error

trend for under-prediction of measured concentrations (see Table 4, below). In view of this, it is unlikely that the poor predictions of simazine in the Hayle catchment are the result of model algorithms. Instead, they are most likely to result from unrepresentatively large values for simazine loadings given in the input data files. Because of the way in which pesticide loadings are calculated from regional survey statistics and interpolated land use data, unrepresentative information is most likely to occur for small catchments and compounds applied mainly to 'minor' crops. Usage of simazine in the Hayle catchment is just such a case.

Although there is insufficient measured data available to carry out meaningful statistical comparisons of measured and predicted concentrations on a catchment by catchment basis, it is possible to make a broad statistical evaluation of model predictions based on weekly data related to positive detections in all catchments. The results are given in Table 4 and shown graphically in ANNEX III.

Table 4. General statistical comparison of measured positive detections vs predicted values for selected pesticides in all test catchments

DataSet	Measured vs predicted linear regression				Scaled RMSE	Model Efficiency
	Straight		Forced through origin			
	equation	r^2	equation	r^2		
All data	y = 0.2821 x + 6.8476	0.4172	y = 0.3036 x	0.4076	1.32	0.1788
Excluding atrazine, chlorfenvinp., γ HCH and endosulfan	y = 0.5264 x +2.8364	0.4633	y = 0.5436 x	0.4623	0.88	0.2727

Two sets of statistics are given in Table 4. The first set gives, for all pesticides with positive detections, the SRMSE, ME, straight linear regression of measured vs. predicted data and linear regression forced through the origin. Although the ME is not unacceptable (*i.e.* a negative value), it is not very good and the SRMSE of 1.32 is poor. Examination of the graphical comparison shows a very consistent under-prediction and the linear regressions show that, on average, predictions underestimate measured data by a factor of 0.3. However, as discussed above, this dataset includes predictions for γ HCH, atrazine, chlorfenvinphos, endosulfan in the Idle and simazine in the Hayle, that for various reasons, would not be expected to give a good comparison with measured data. A second dataset, excluding these compounds was therefore statistically analysed and the results are also given in Table 4 and ANNEX III. For this dataset, both the ME and SRMSE have improved significantly, and are well within the 'acceptable' range, although neither can be said to be good. Overall model prediction has improved, but there is still a very consistent trend of under-prediction by a factor of 0.54.

There are two likely reasons for the dominant under-prediction of measured concentrations, both related to the use of monthly pesticide loadings as input data. Firstly, the way in which the monthly pesticide loadings input data are calculated, is likely to significantly under-estimate actual loadings to intensive arable areas of a catchment. Such areas are likely to contribute disproportionately to catchment water residues and the model will thus under-estimate such residues. Secondly, the way in which the model converts monthly pesticide loadings into weekly values may also underestimate actual weekly loadings. Although, as discussed in section 2.3.1, the model attributes half of the monthly loading to a single week, on some occasions, particularly in small catchments, this may still significantly underestimate the actual weekly loading. In order to confirm these suggested reasons, an investigation should be carried out into how well national pesticide loadings data represent actual loadings within a range of agricultural catchments.

Overall, the general data comparison and statistical analysis suggest that, for diffusely-applied agricultural pesticides, the model will give acceptable results. For such compounds, maximum concentrations within catchments are, on average, likely to be twice the predicted maximum values. Model simulations for compounds with significant non-agricultural usage, or with a 'minor crop' usage in small catchments, are unlikely to be representative.

4.   CONCLUSIONS AND RECOMMENDATIONS

The catchment scale model described in this report has been tested against a range of measured river flow and pesticide concentration data in a range of catchments representing a variety of sizes, agricultural situations, climatic and hydrogeological conditions within England and Wales. The model has been shown to give acceptable predictions of both flows and pesticide concentrations for most of the representative catchments studied. Because of its semi-empirical approach based on national scale relationships, detailed parameter estimation and model calibration on a catchment by catchment basis are unnecessary. The model is thus likely to be robust, at least when used within the UK.

When applying the model, the following conclusions should be borne in mind:

- **Flows in dominantly 'impermeable' catchments are likely to be under-estimated.**

- **Flows in dominantly 'permeable' catchments are likely to be over-estimated**

- **Flow predictions for chalk and chalky till catchments in E. Anglia should be treated with caution.**

- **Flow predictions for catchments with complex interbedded Jurassic limestone/ironstone and clay lithologies are likely to be very poor, particularly where the catchment is less than about 300 sq. km. in size.**

- **The model is unlikely to give reasonable predictions of concentrations for pesticides with a significant non-agricultural usage**

- **Predictions of catchment concentrations from diffusely applied agricultural pesticides are likely to be about half of the actual peak concentrations.**

- **Predictions of concentrations from pesticides with a dominantly 'minor crop' usage pattern should be treated with caution, especially within catchments less than about 300 sq. km. in size.**

- **All predictions on small catchments, less than about 300 sq. km. in size, should be treated with caution.**

- **All predictions on catchments with a significant urban component should be treated with caution.**

In addition, it is recommended that the following possibilities for further evaluation and improvement of model predictions be investigated:

- **Proper statistical evaluation of predicted concentrations for at least 2 diffusely applied agricultural pesticides in at least 2 catchments (one**

permeable and one impermeable), using a comprehensive measured dataset comprising at least one measurement per week.

- Improvement of the spatial resolution for Rainfall and Hydraulically Effective Rainfall

- Investigation of how well the national Monthly Pesticide Loadings datasets represent actual agricultural pesticide usage in a range of agricultural catchments.

- Refinement of the SWATCATCH model by developing soil-related, hydrogeological-specific 'f' factors for calculating base flows.

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ANNEX I

MODEL INPUT AND OUTPUT FORMATS

MODEL INPUT FORMAT SPECIFICATION FOR SWATCATCH

1	Catchment area, **Ac** (ha)	(f8.1)
2	Number of 2km x 2km grids, **y**, in catchment	(i6)
3	Number of years, **N**, to be run through the model	(i6)
4	For specified pesticide, ONE record in format	(4e12.5)

Koc (l/kg); ⟵——

T$_{1/2}$ (days); ⟶

Solubility **S** (mg/l); ——

Henrys constant **Kaw** (dimensionless) ——

5 For each 2km x 2km grid

Depth to saturated zone, **Dz** (m)	(f6.1)
Fraction of grid in catchment, **fract.g**	(f6.2)
Number of soil series, **n**, in grid	(i6)
Long term average annual HER, **AAHER** (mm)	(f6.1)
MORECS effective weekly rainfall, **HER** (mm)	(13f6.1)
	(4*N such lines)
MORECS total weekly rainfall, **R** (mm)	(13f6.1)
	(4*N such lines)
Monthly pesticide loadings, **PL** (kg)	(12e12.5)
	(N such lines)

6 For each soil series in turn, ONE record in format   (3f6.2,2f6.1,i6)
comprising -

Fraction of soil series, **fract.s** in grid;

Base flow Index, **BFI**;

Intermediate runoff fraction, **IRF.**

SPR (%);

Minimum standard rainfall volume **MSRV** (mm);

Number of soil layers, **v**;

7 For each soil layer in turn, ONE record in format: (3f6.1,f6.2,4f6.1,f6.2)
comprising -   (v such lines)

upper depth, **UD** (cm);

lower depth, **LD** (cm);

organic carbon, **OC** (%);

bulk density, **Db** (g/cc);

total pore space, **T** (% vol);

water content at 5 kPa, **θ5** (% vol);

water content at 200 kPa, **θ200** (% vol);

water content at 1500 kPa, **θ1500** (% vol)

Conductivity at 5 kPa, **Kθ5** (cm / day)

(**n** combinations of 6 and 7)

(**y** combinations of 5, 6 and 7)

MODEL OUTPUT FORMAT SPECIFICATION FOR SWATCATCH

For each year of simulation (**N** years)

Year	(i6)
Weekly mean flows, **Fc** ($m^3 s^{-1}$) (52 values)	(13e14.6)
Weekly base flows, **Bc** ($m^3 s^{-1}$) (52 values)	(13e14.6)
Weekly average pesticide concentration, **CM** (ng l^{-1}) (52 values)	(13e14.6)
Weekly peak pesticide concentration, **CP** (ng l^{-1}) (52 values)	(13e14.6)

ANNEX II

COMPARISONS OF MEASURED AND SIMULATED FLOWS FOR TEST CATCHMENTS

Measured vs Predicted flows for all catchments
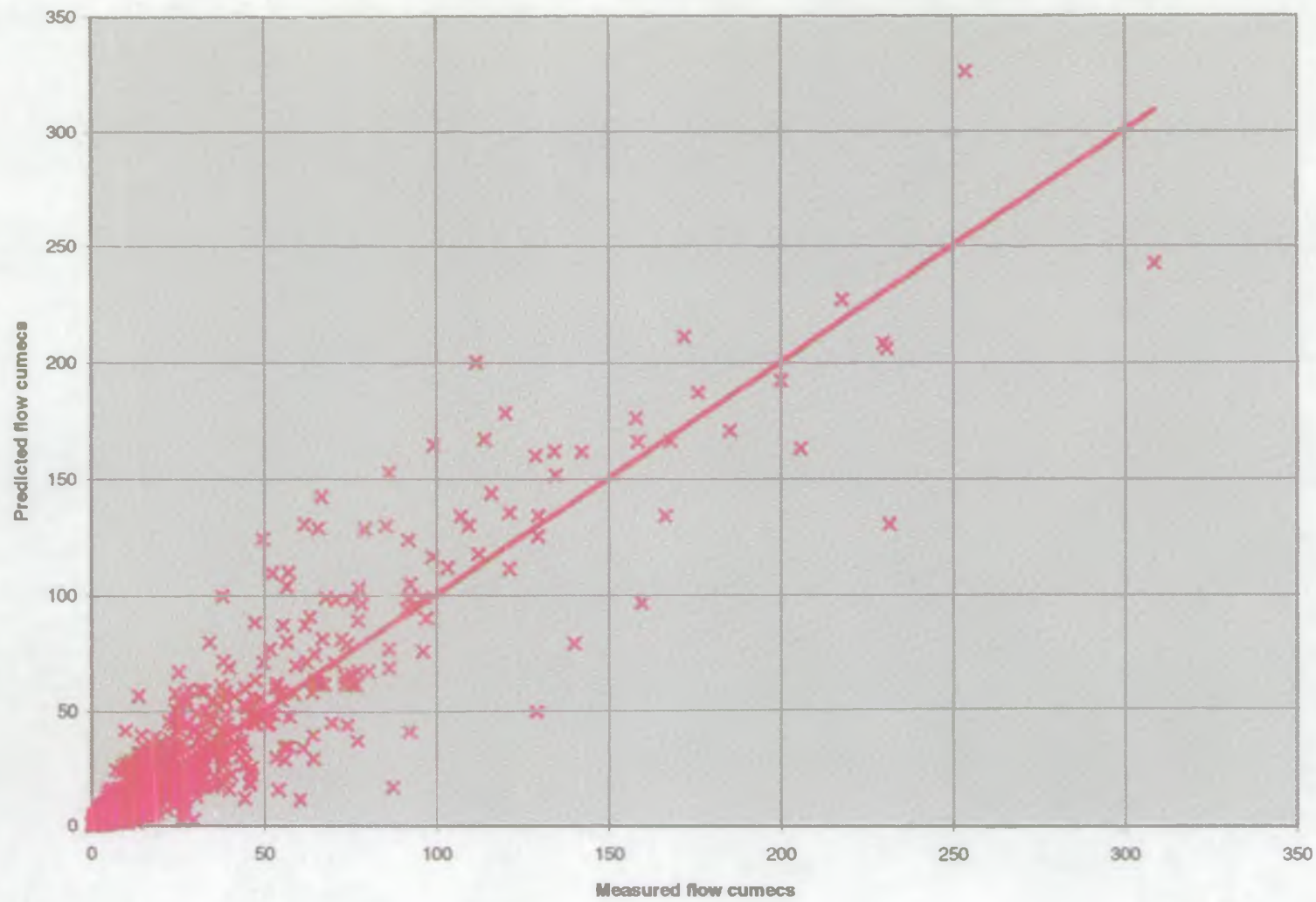
$y = 0.9999x + 0.3145$
$R^2 = 0.8733$

TEST CATCHMENTS 8 + 9

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

9

RIVER WENSUM
034011

NAR
033058

32007

8

TF724D012000

34011

34014

WENSUM

TG1648013240
TG1630013120
TG1622013230

TG2100009700
TG2060009500
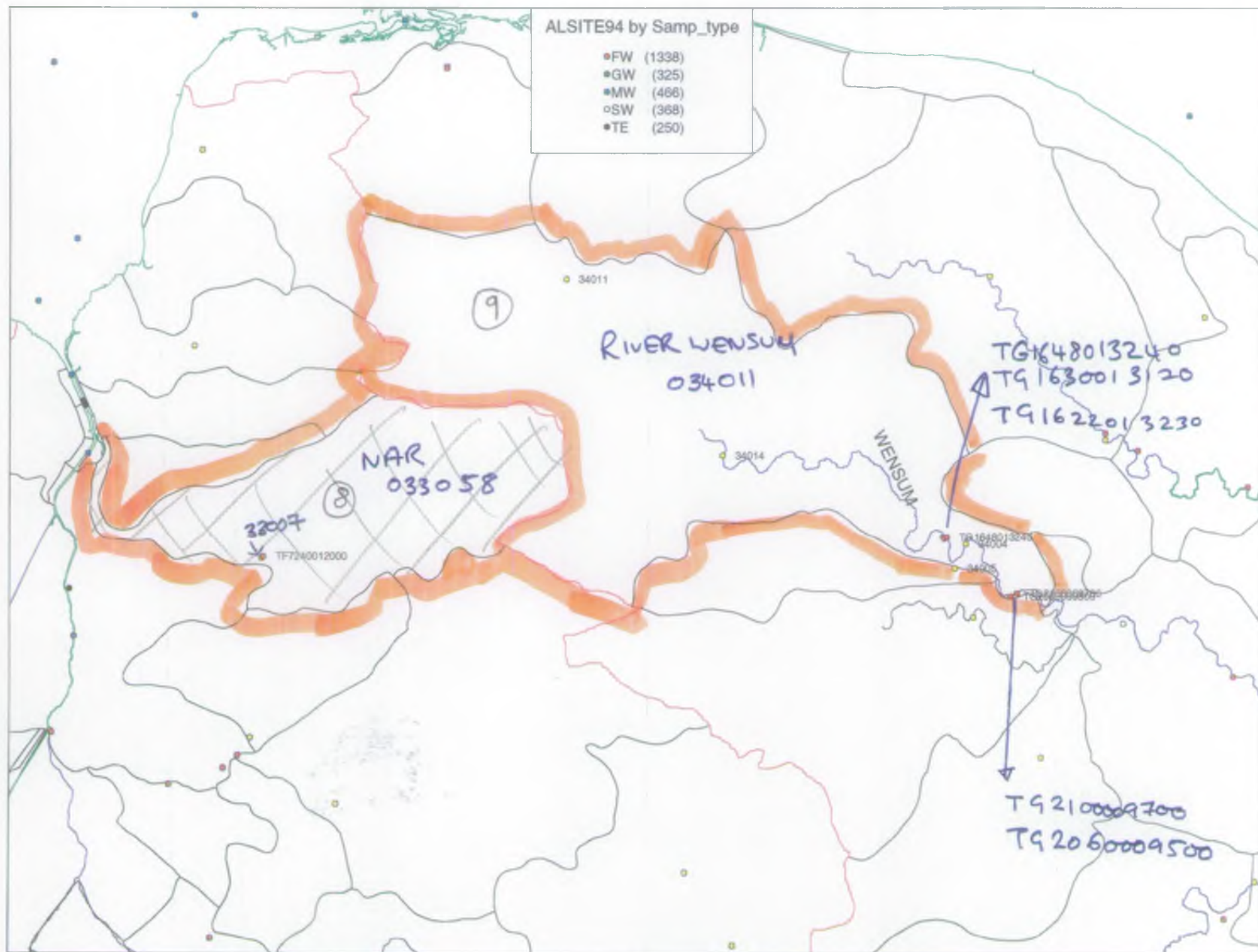
R. Wensum 1992-94 weekly flows
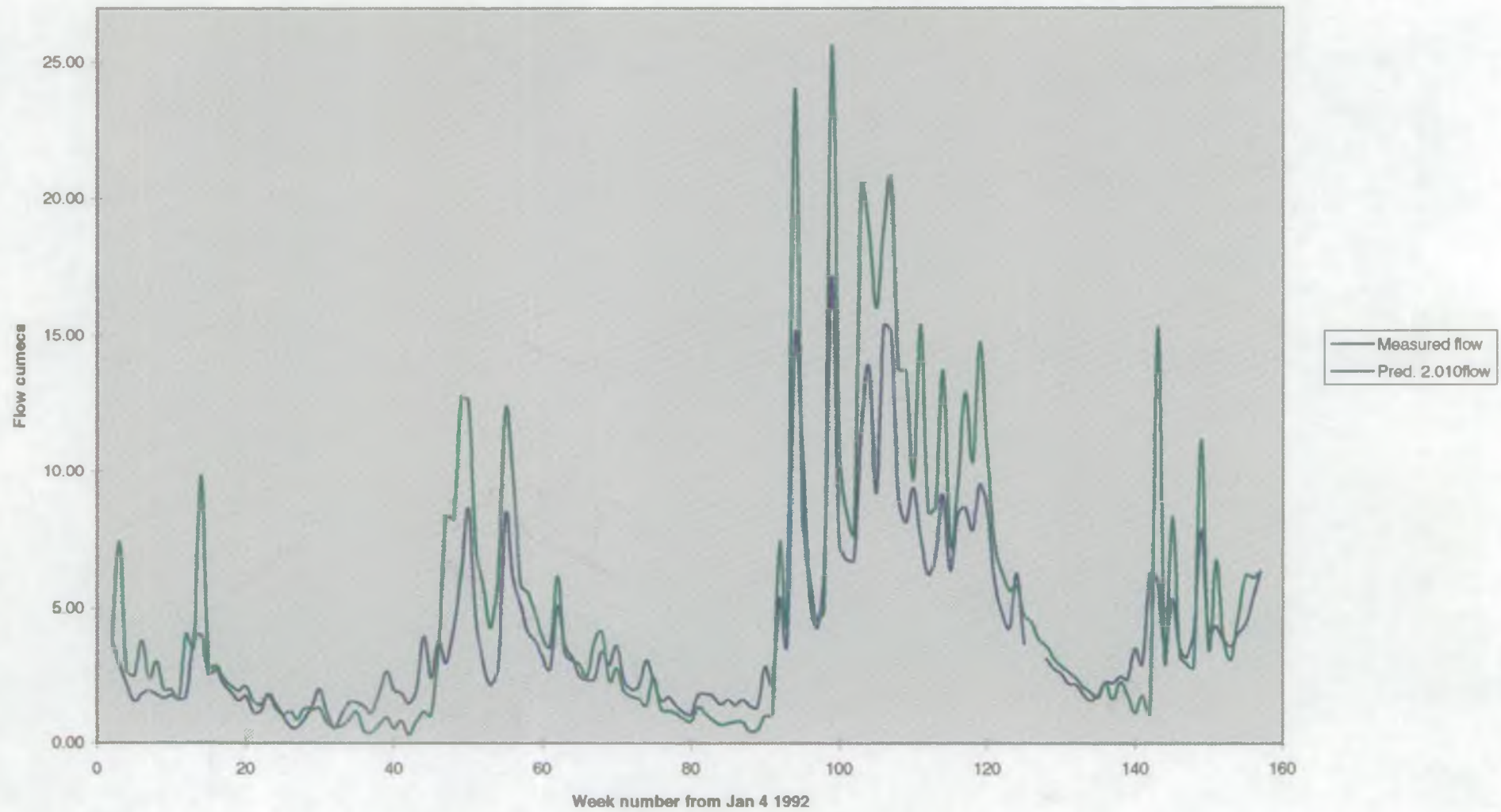
R. Wensum Measured vs Predicted flow data
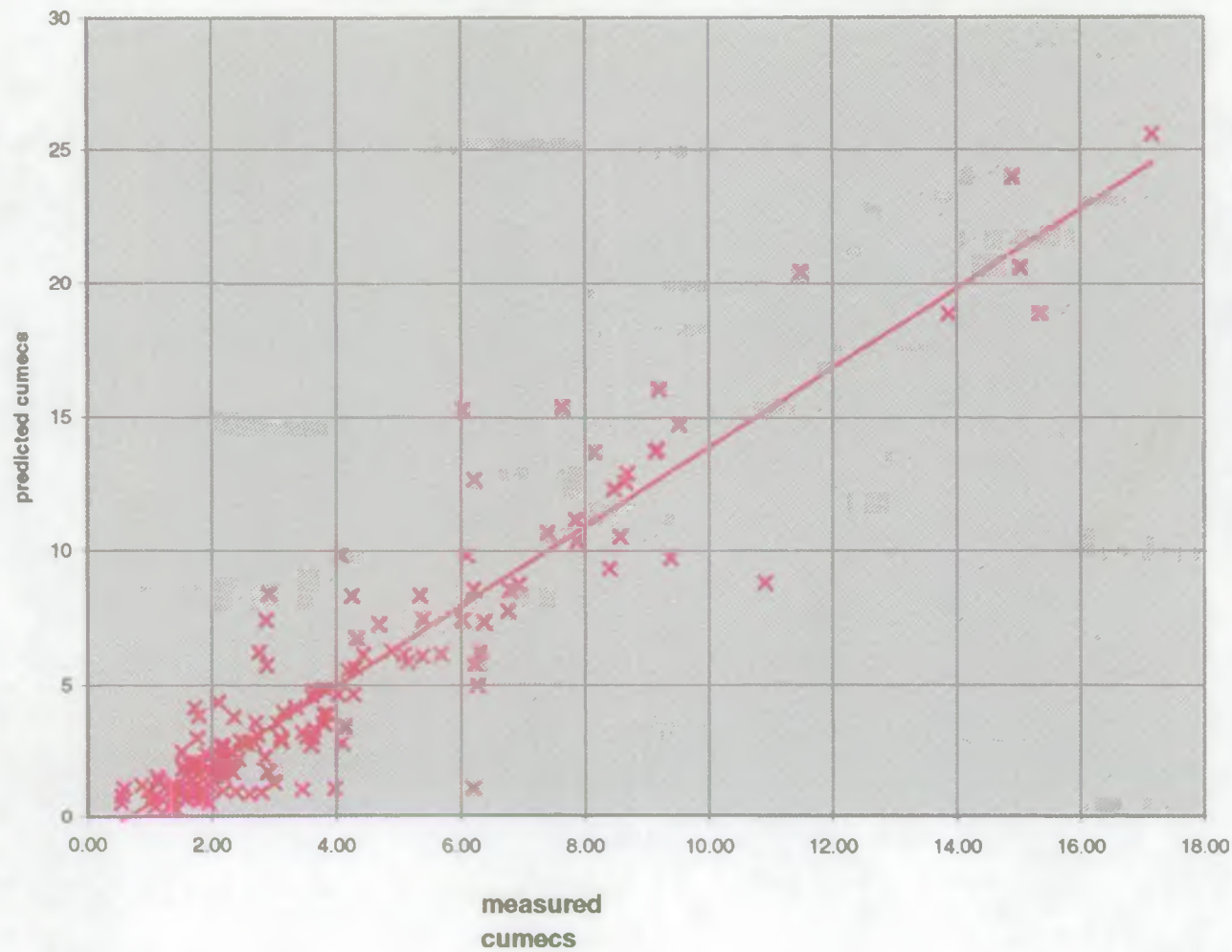
$y = 1.4839x - 0.9653$
$R^2 = 0.8719$

TEST CATCHMENT 1

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

RIVER COQUET
022006A

COQUET

RIVER COQUET
022006B

COQUET

22009

22001

ND370006100

R. Coquet 1992-94 flows

Week number from Jan 4 1992

Flow cumecs

Meas. flow
Predicted flow 0.2,10
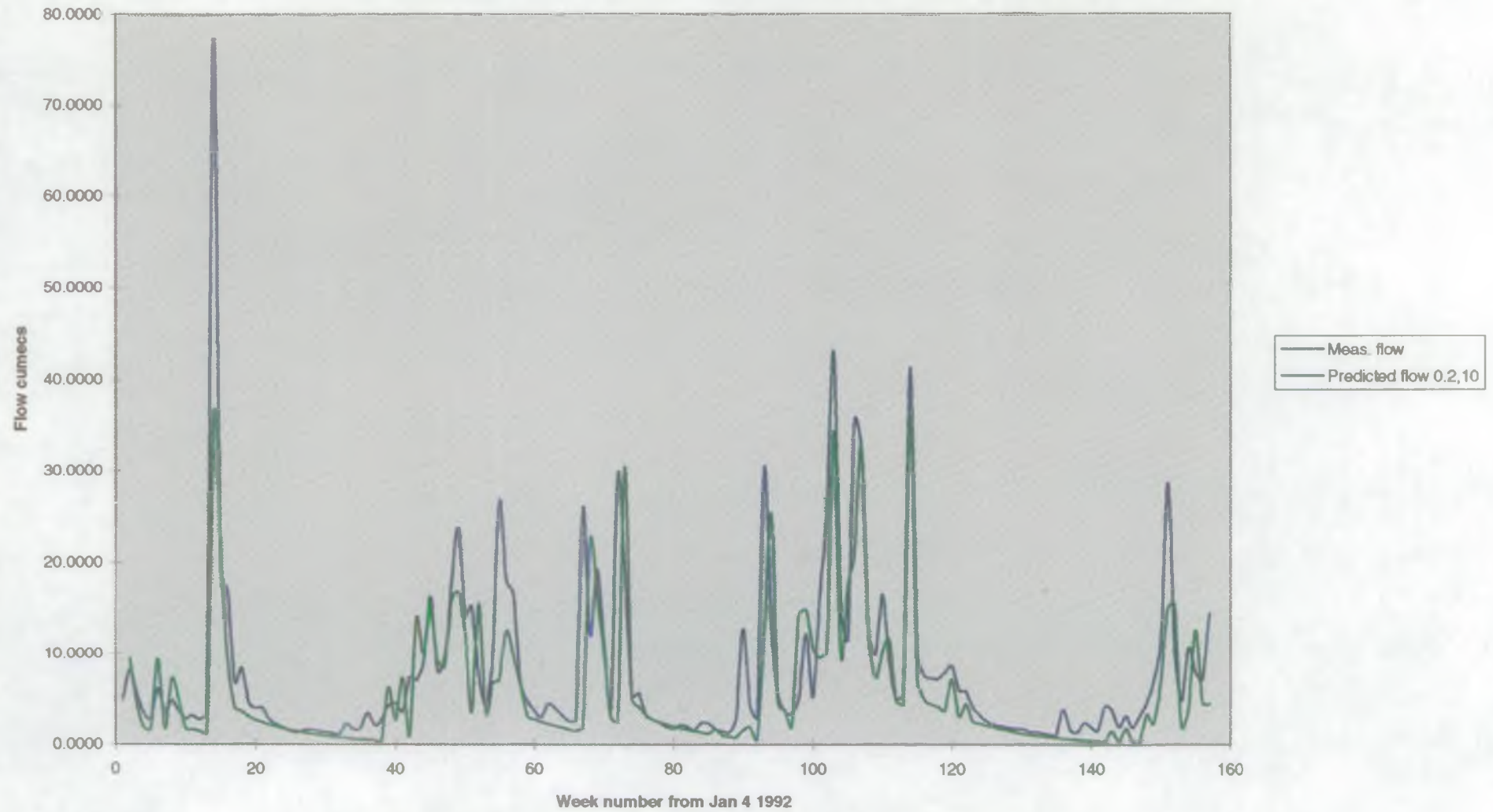
R. Coquet measured vs predicted flows
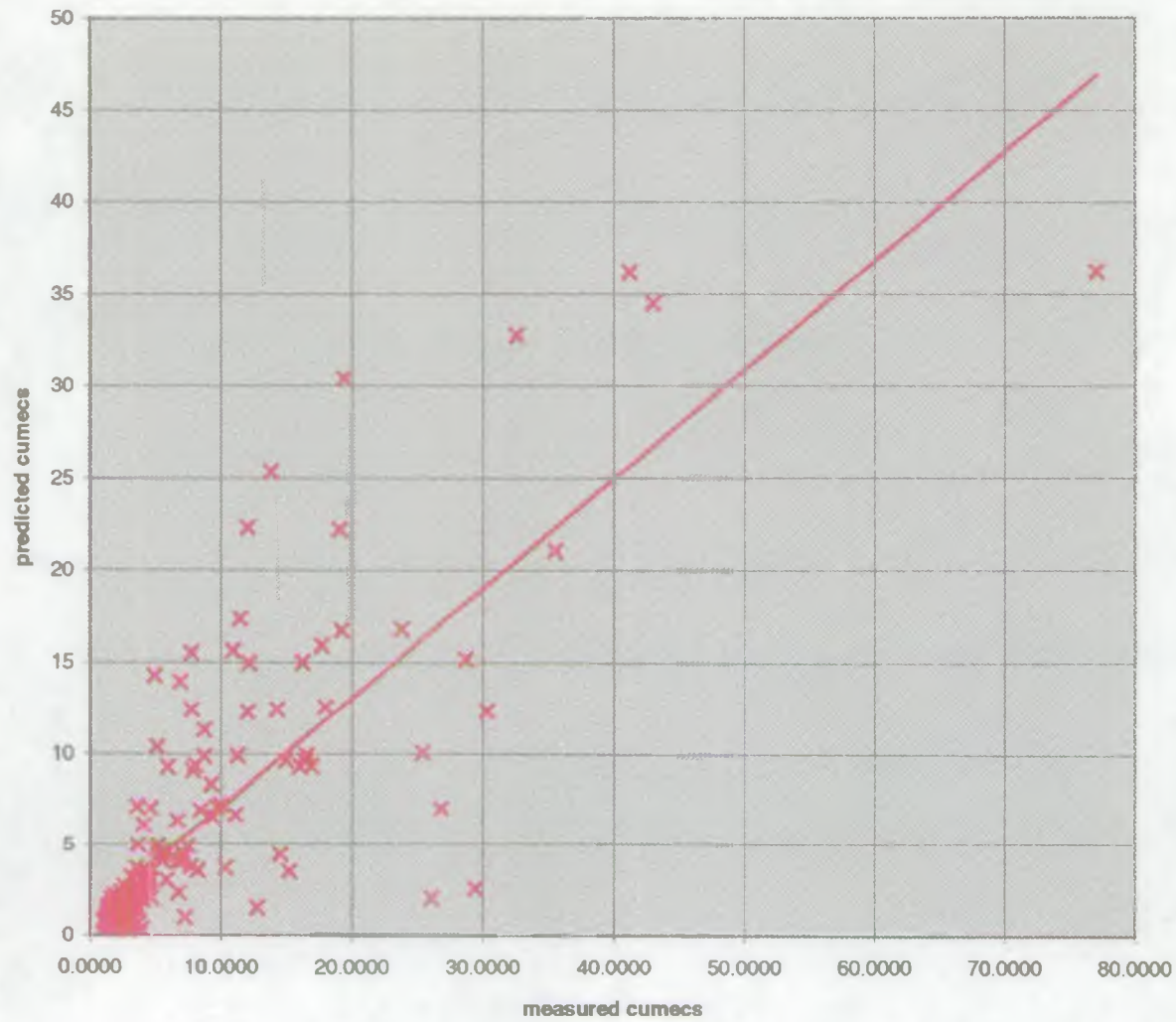
$y = 0.5935x + 1.1593$
$R^2 = 0.634$

TEST CATCHMENT 15

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

UPPER
STOUR
043031

CALE
043032

LYDDEN
043033

MIDDLE
STOUR
043034

← STOUR

ALLEN
043035

MOORS
043036

LOWER
STOUR
043037

SZ137 0093700
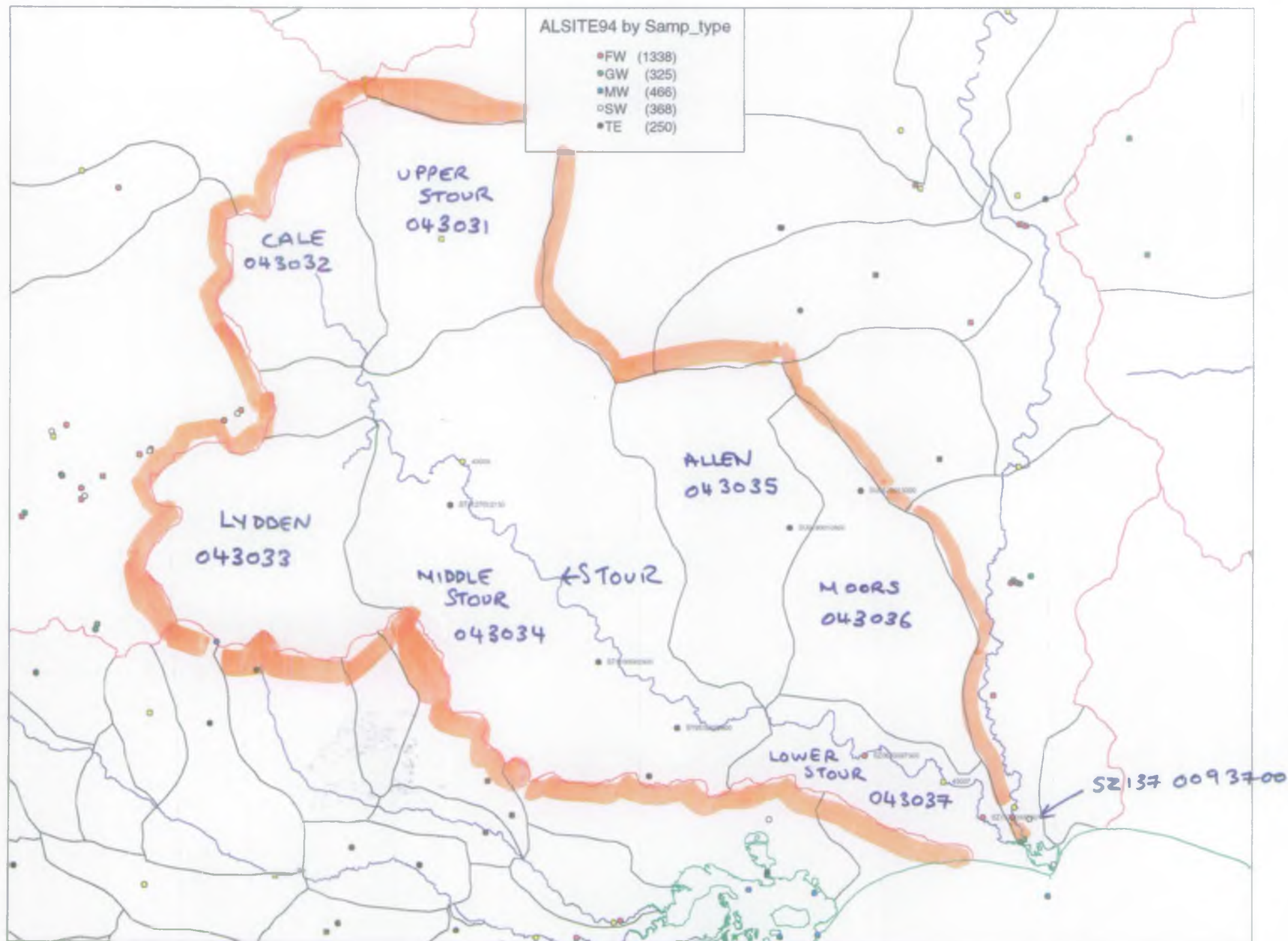
R. Stour weekly flows 1992-94
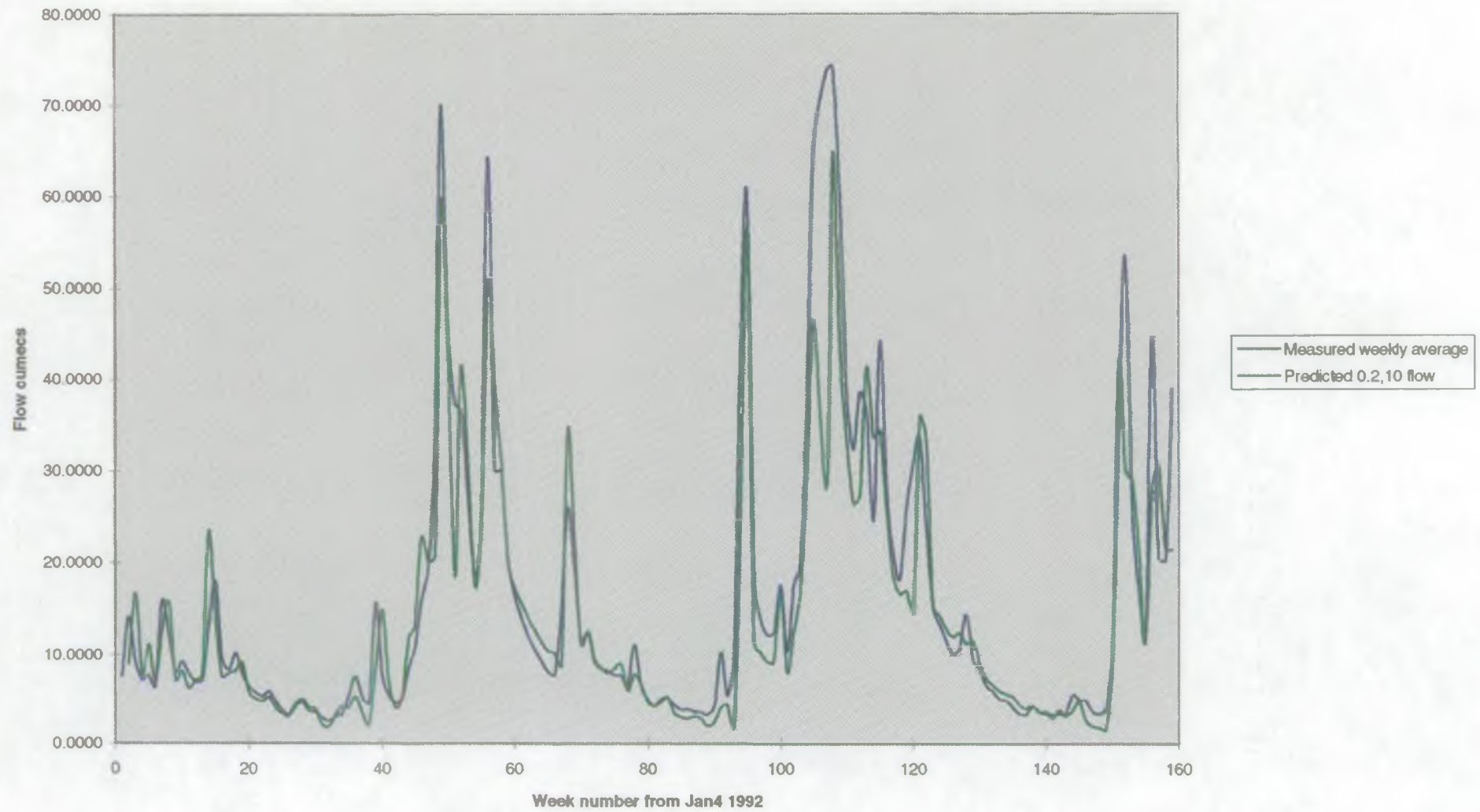
Hants. Stour measured vs predicted flows

$y = 0.6482x + 4.0118$
$R^2 = 0.6116$

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

SK7660096200

SK6560092700

28015

28047 28091

IDLE TO RYTTON CONFLUENCE 028074

IDLE

28049

28036

RIVER POULTER 028073

28044

MEDEN, MAUN TO POULTER CONFL 028072

28032

MEDEN TO CONJURE ALDERS 028071

MAUN TO CONJURE ALDERS 028070
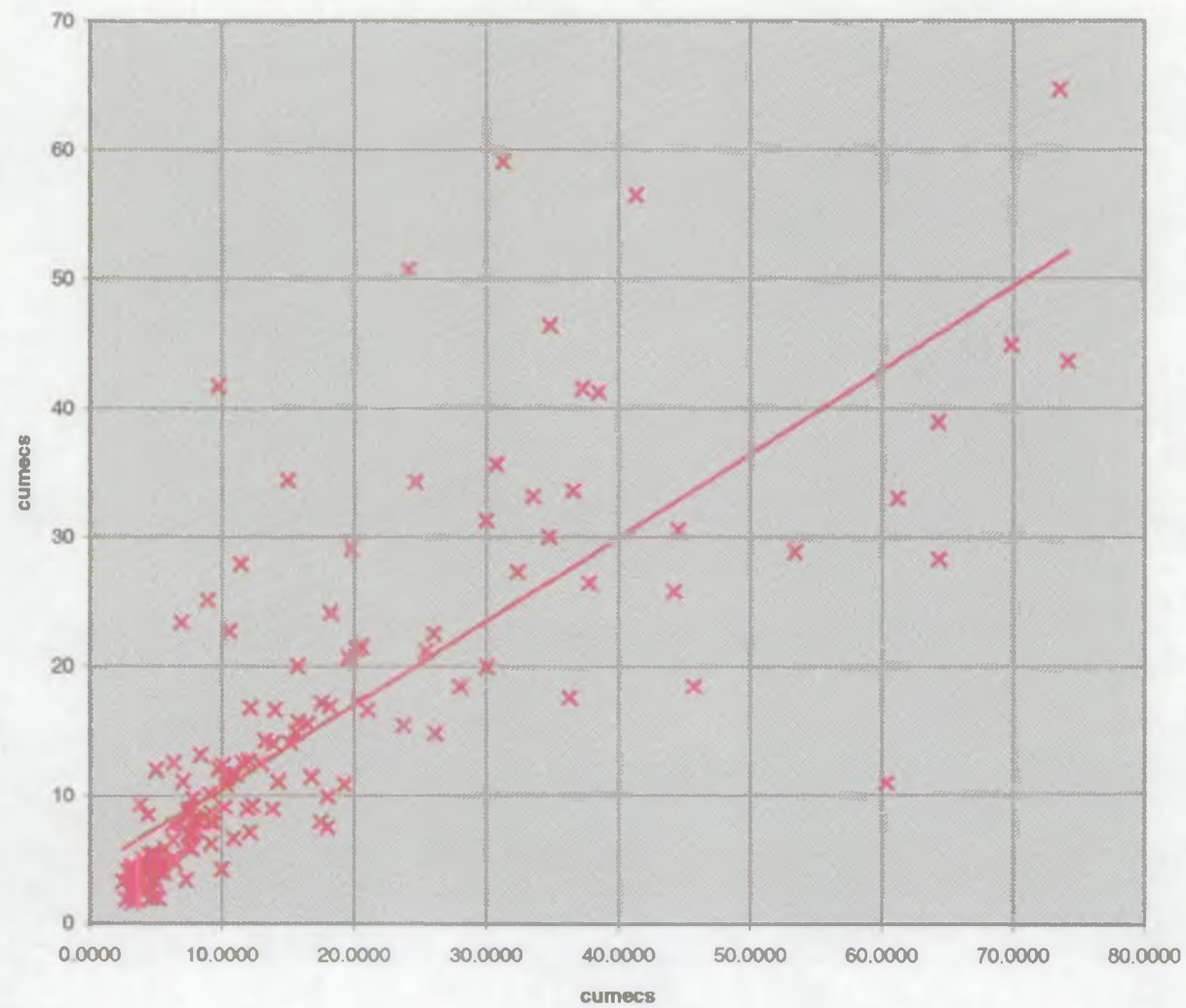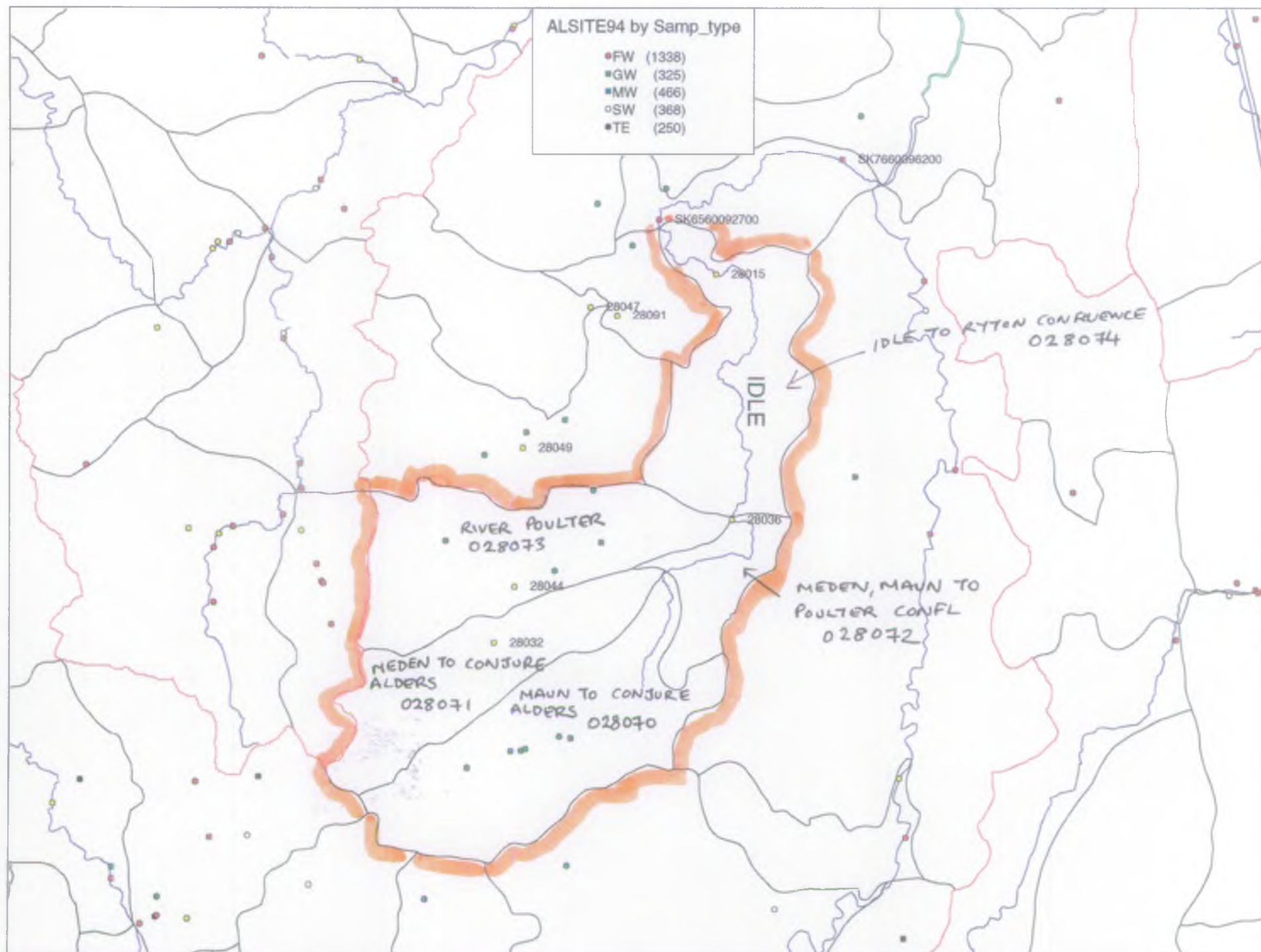
R. Idle weekly flows 1992-94

R. Idle measured vs. Predicted flows

$y = 1.3319x - 1.0571$
$R^2 = 0.7235$

Predicted flow oumecs

Measured flow cumecs

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

STOUR
(WORCESTERSHIRE)
054006

SO8295079150

SO8305076850

SO8310075700

SO8305074650

SO8256073750

SO8255072750
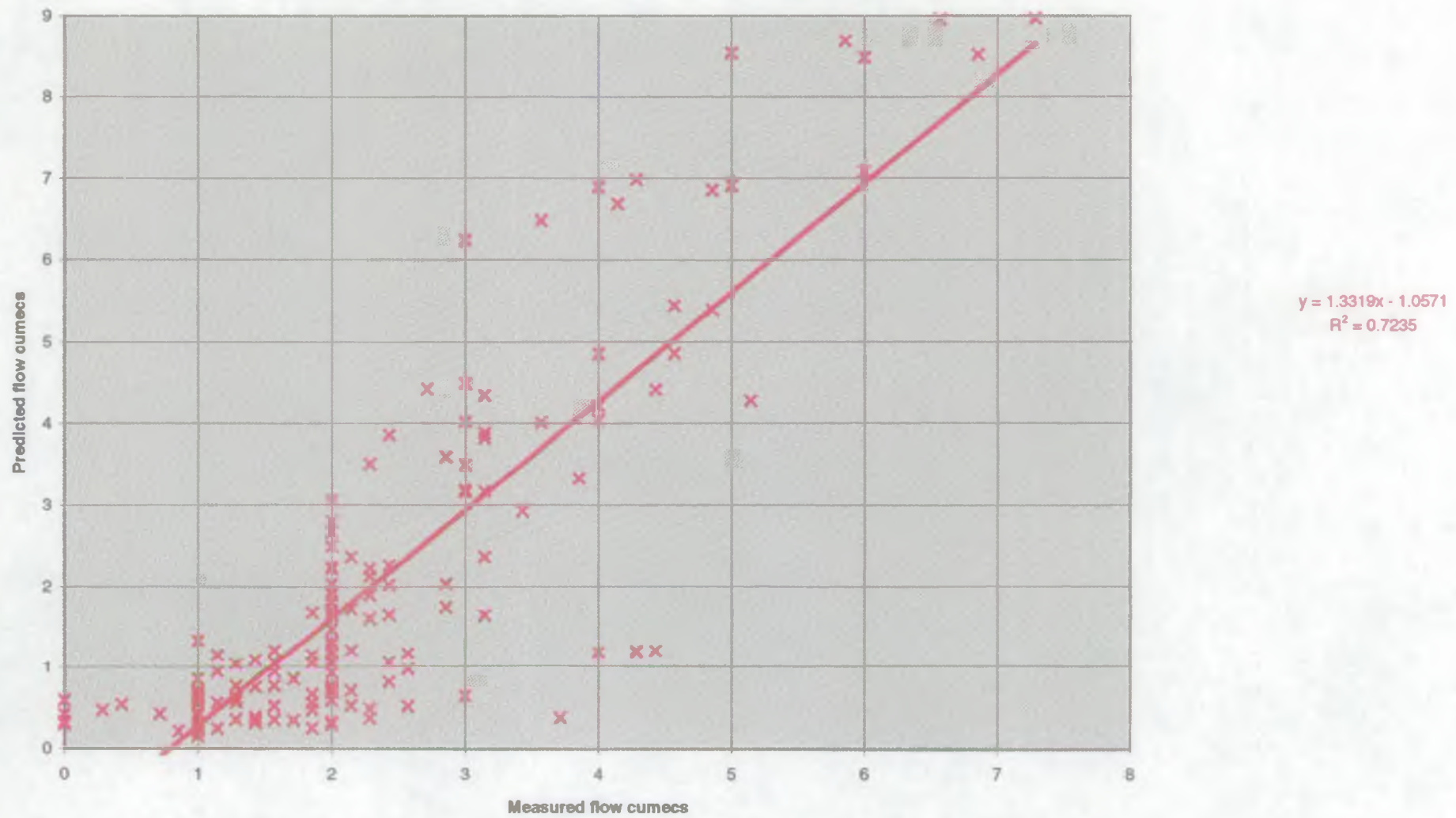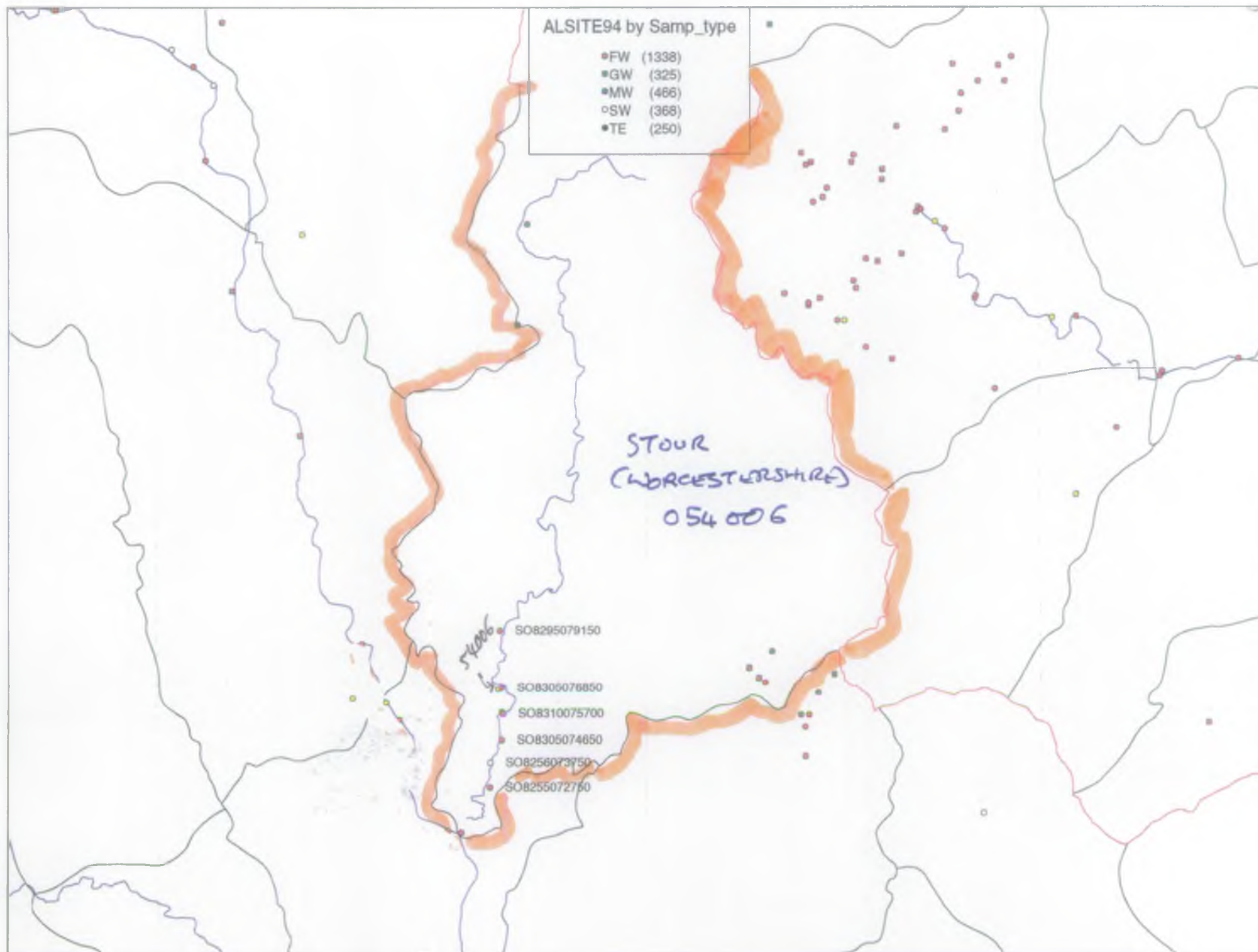
R. Stour (Worcs.) weekly flows 1992-94

Flow cumecs

Week number from Jan 4 1992

Measured average flow
Predicted 0.2,10flow

Worcs. Stour measured vs. predicted flows

$y = 1.2051x - 0.2059$
$R^2 = 0.498$

measured cumecs

predicted cumecs

TEST CATCHMENT 5

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

028026

SJ9954008700

028025

028030

028028

28061   028027   028029

SK1460050400

28098

028032   DOVE

028031   028034

28608

028033

028035

28018

SK2680027000

R. Dove weekly flows 1992-94

Week number from Jan 4 1992

R. Dove measured vs. predicted flows

$y = 0.5097x + 1.0662$
$R^2 = 0.6123$

ALSITE94 by Samp_type
- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

RIVER NENE (WHILTON BRIDGE) 032001

NENE

RIVER LEAM 054012

WOOTON BROOK KIS'BRY 032004

RIVER NENE KIS'BRY BRIDGE 032002

CHERWELL

SP4517070250
SP3485068920
SP4070068200
SP4050068800
54040
SP3310065700
SP4199064660
11
SP3895056750
SP4470053010
12
33056
32006
32001
33018

R. Leam weekly flows 1992-94

R. Leam Measured vs. Predicted flows

$$y = 0.7778x + 0.3258$$
$$R^2 = 0.6246$$

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

062003

062002

TEIFI

062001

SN7800067500
SN7910066700

SN2180043640

 flood

SN 2280043500

SN491006900
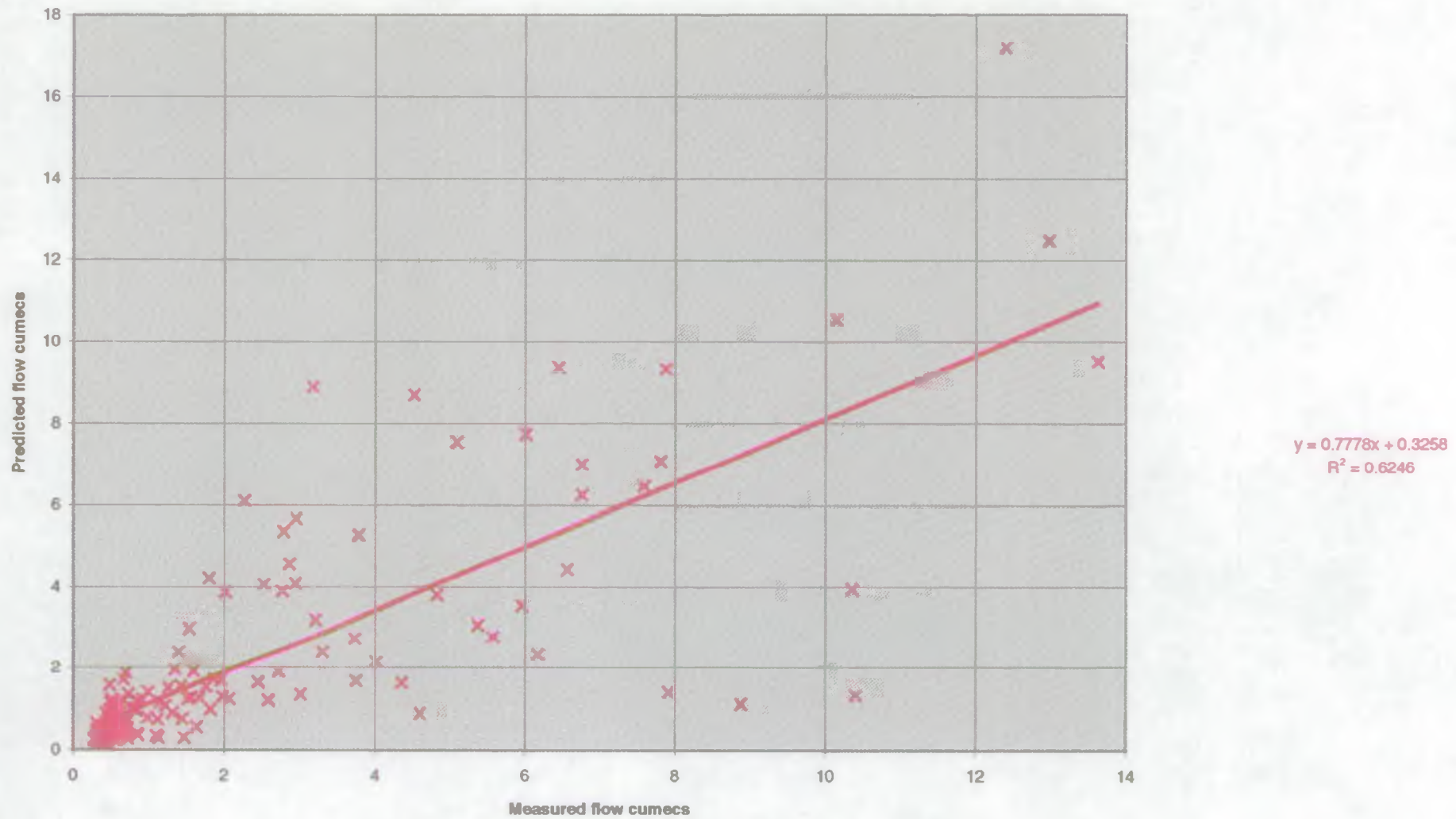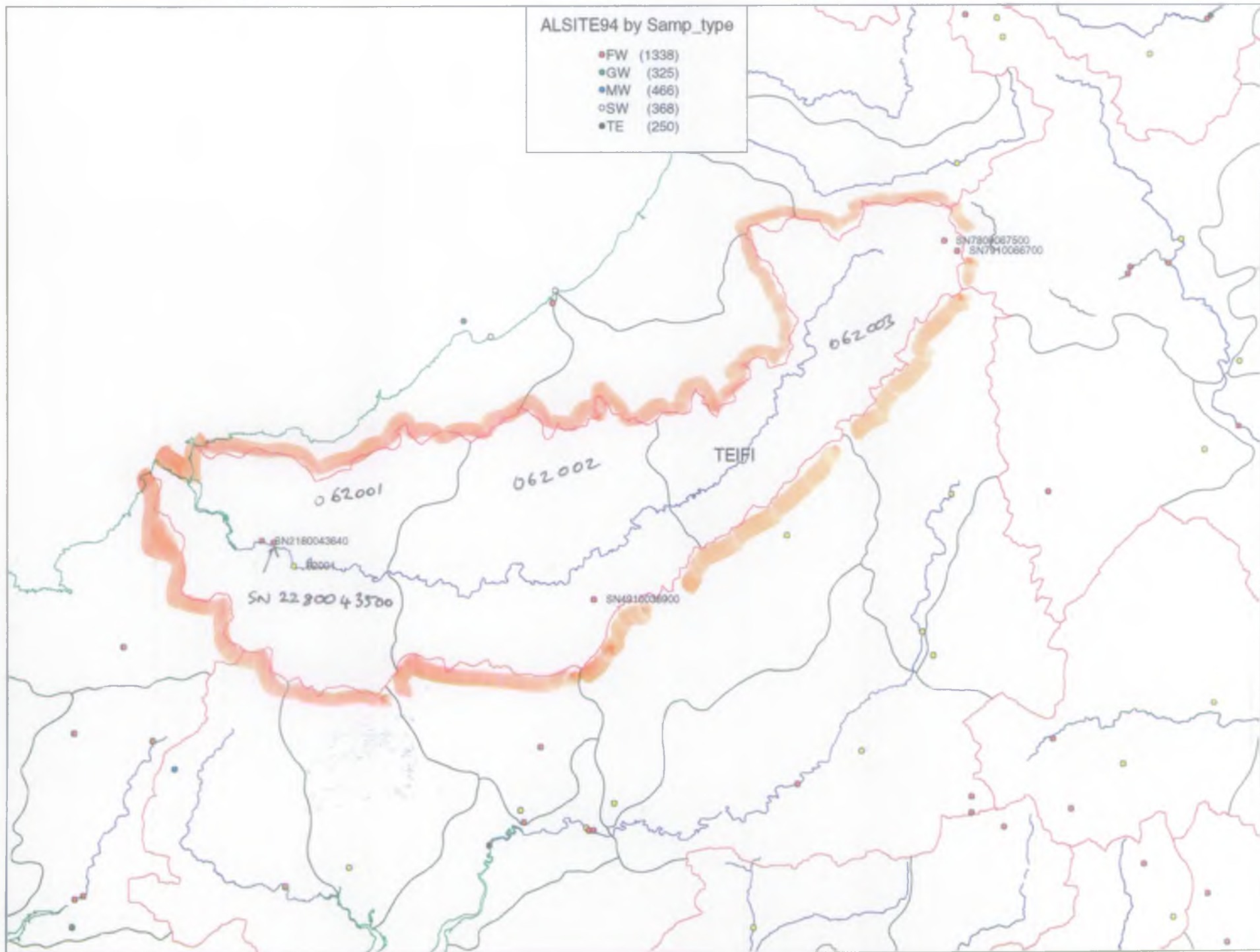
R. Teifi Weekly flows 1992-94

Flow cumecs

Week number from Jan 4 1992

Measured flow
Pred. 0.2,10 flow
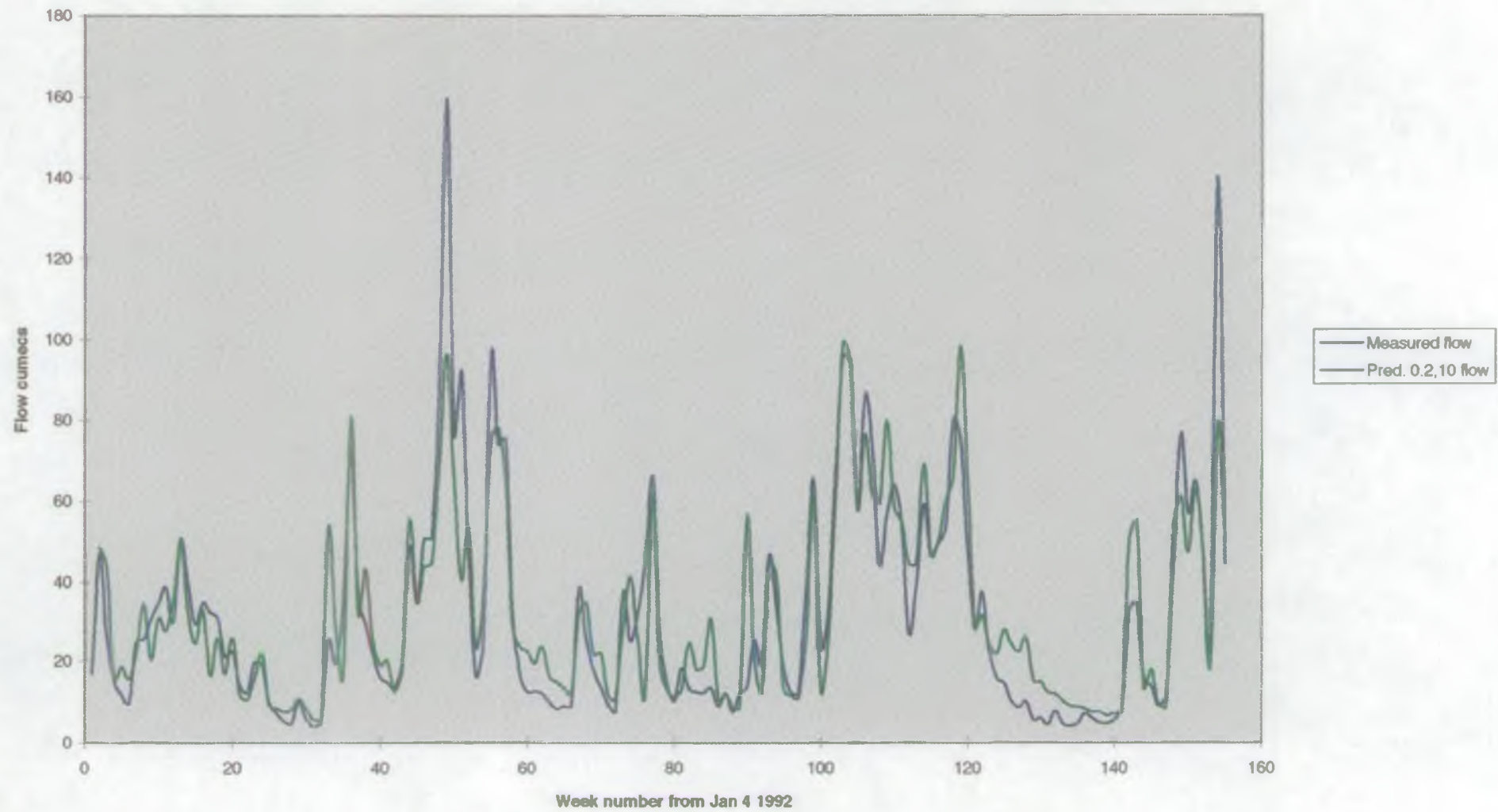
R. Teifi Measured vs. Predicted flows

$y = 0.6992x + 9.8808$
$R^2 = 0.7459$

Predicted flow cumecs

Measured flow cumecs

TEST CATCHMENT 3

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

? 07 1002

DARWEN

SD5570927968

71013   SD6940028200
SD7020025900

SD6780022200
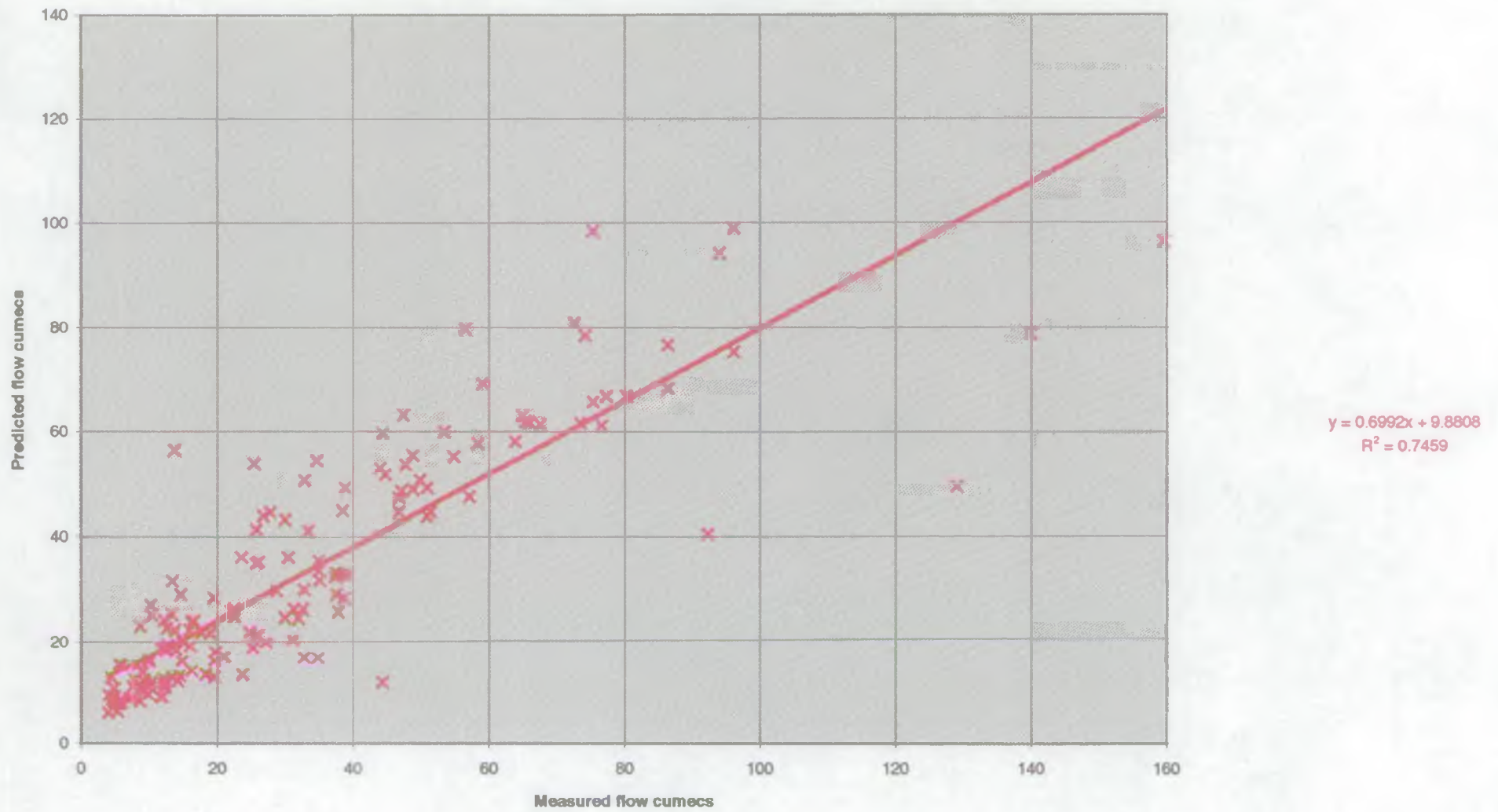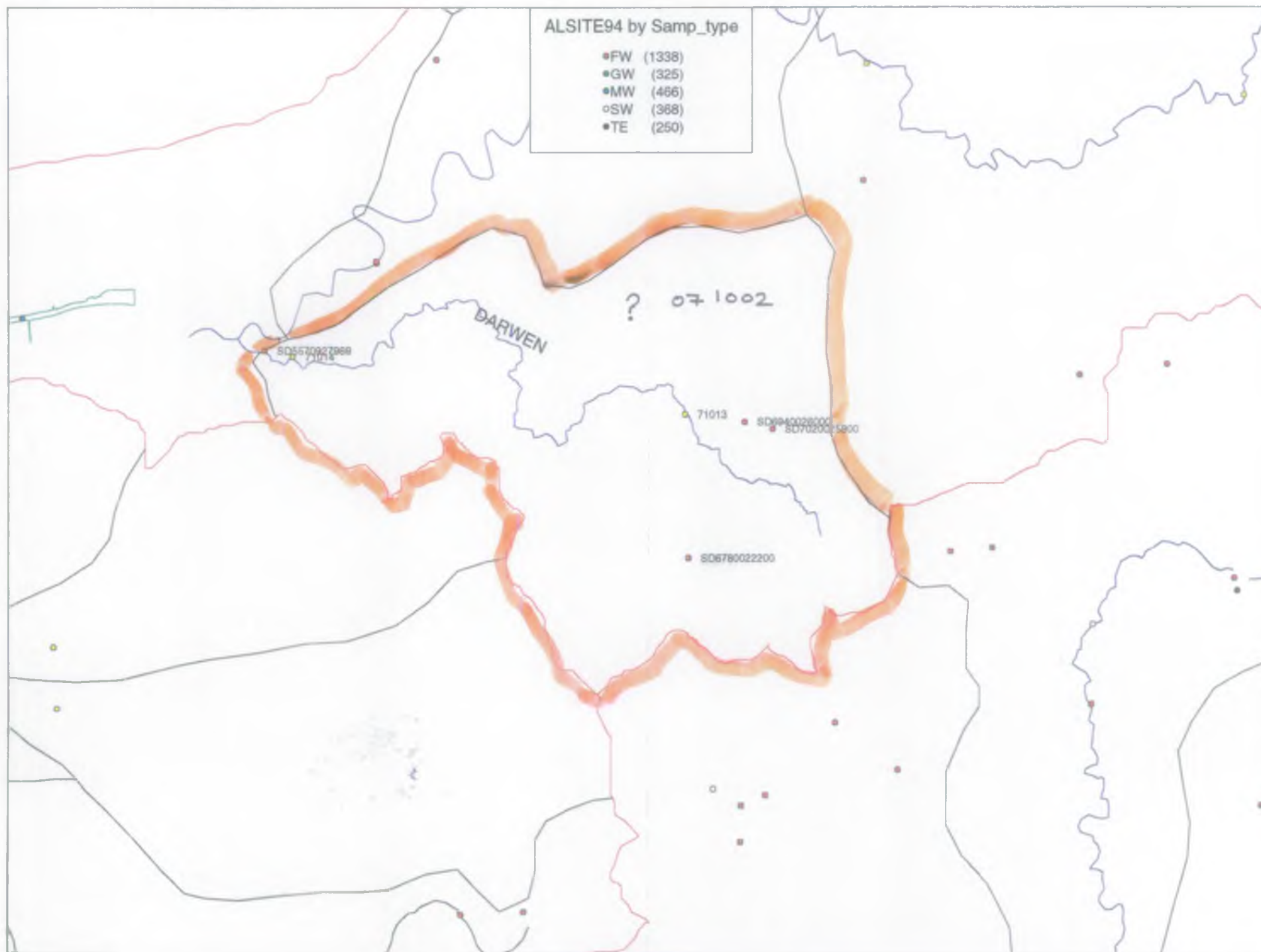
R. Darwen weekly flows 1992-94

Flows cumecs

Week number from Jan 4 1992

Measured flow
Predicted 0.2,10 flow
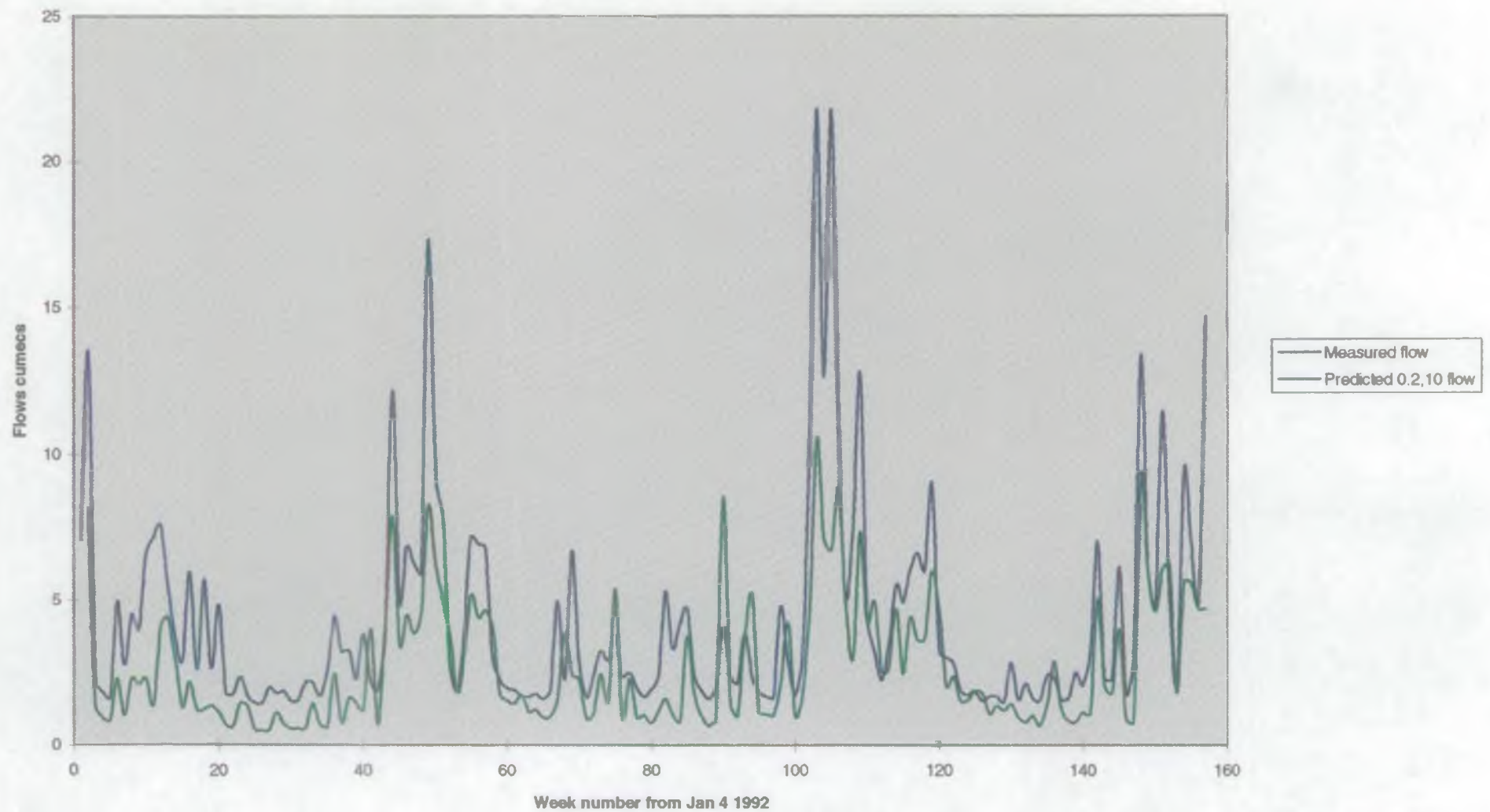
R. Darwen measured vs. Predicted flows

$y = 0.4776x + 0.6435$
$R^2 = 0.6495$

Predicted flow cumecs

Measured flow cumecs

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

RIVER NENE (WHILTON BRIDGE)
032001

NENE

RIVER LEAM
054012

WOOTON BROOK
KIS'BRY
032004

RIVER NENE
KIS'BRY BRIDGE
032002

CHERWELL

R. Nene weekly flows 1992-94

Flow cumecs

Week number from Jan 4 1992

- Measured flow
- Predicted 0.2,10flow
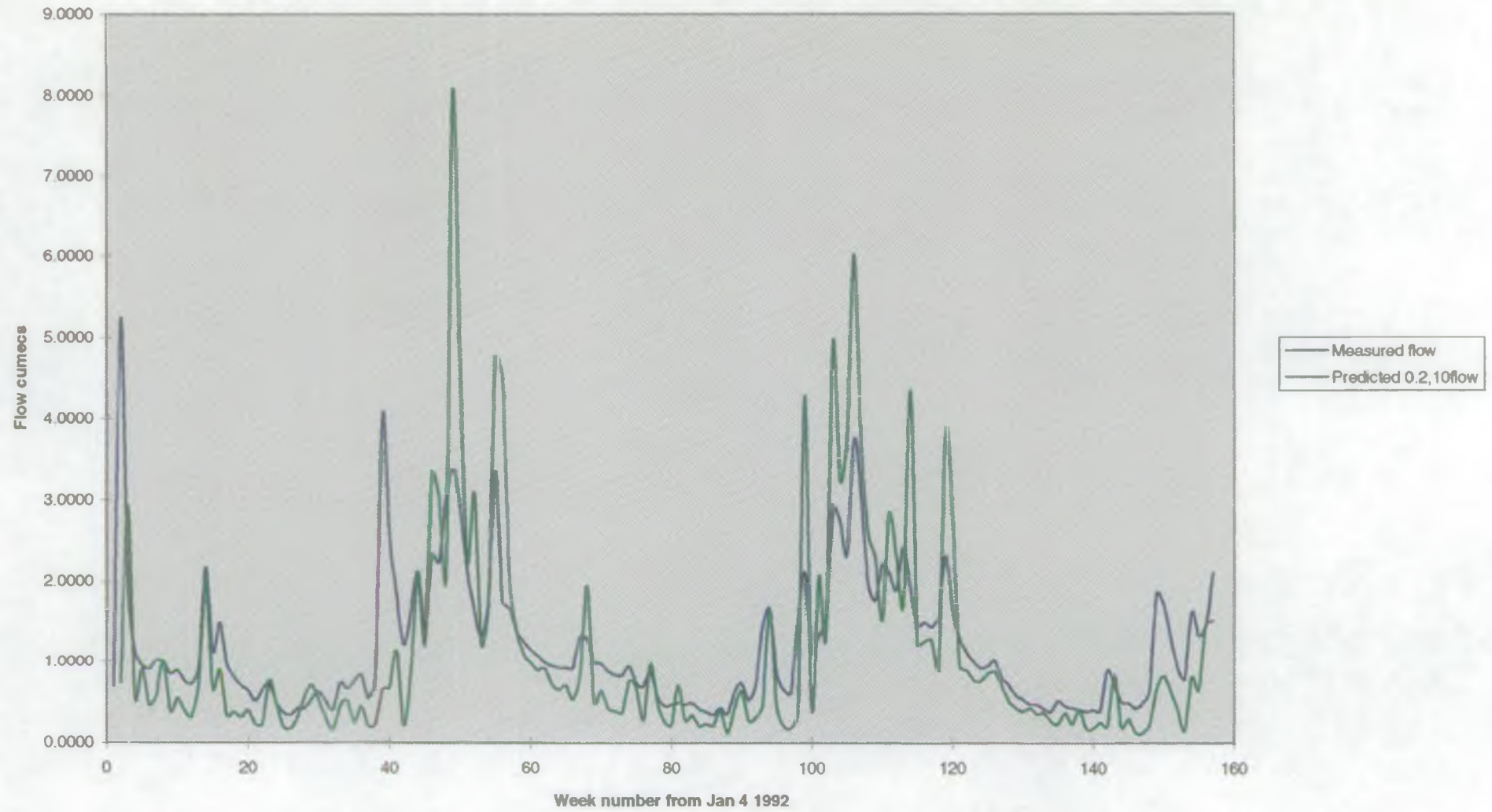
R. Nene measured vs. predicted flows

$y = 1.131x - 0.2575$
$R^2 = 0.5313$
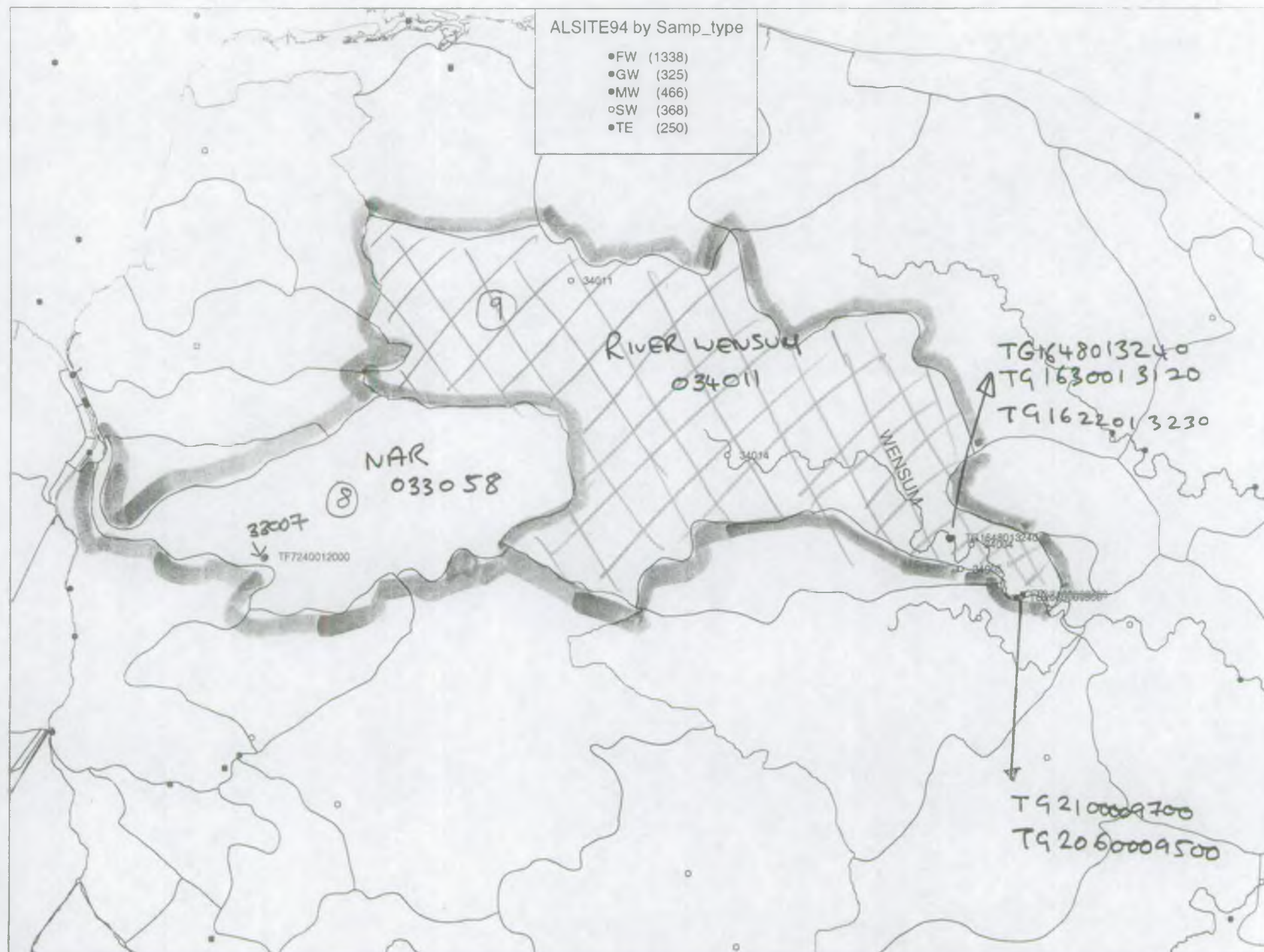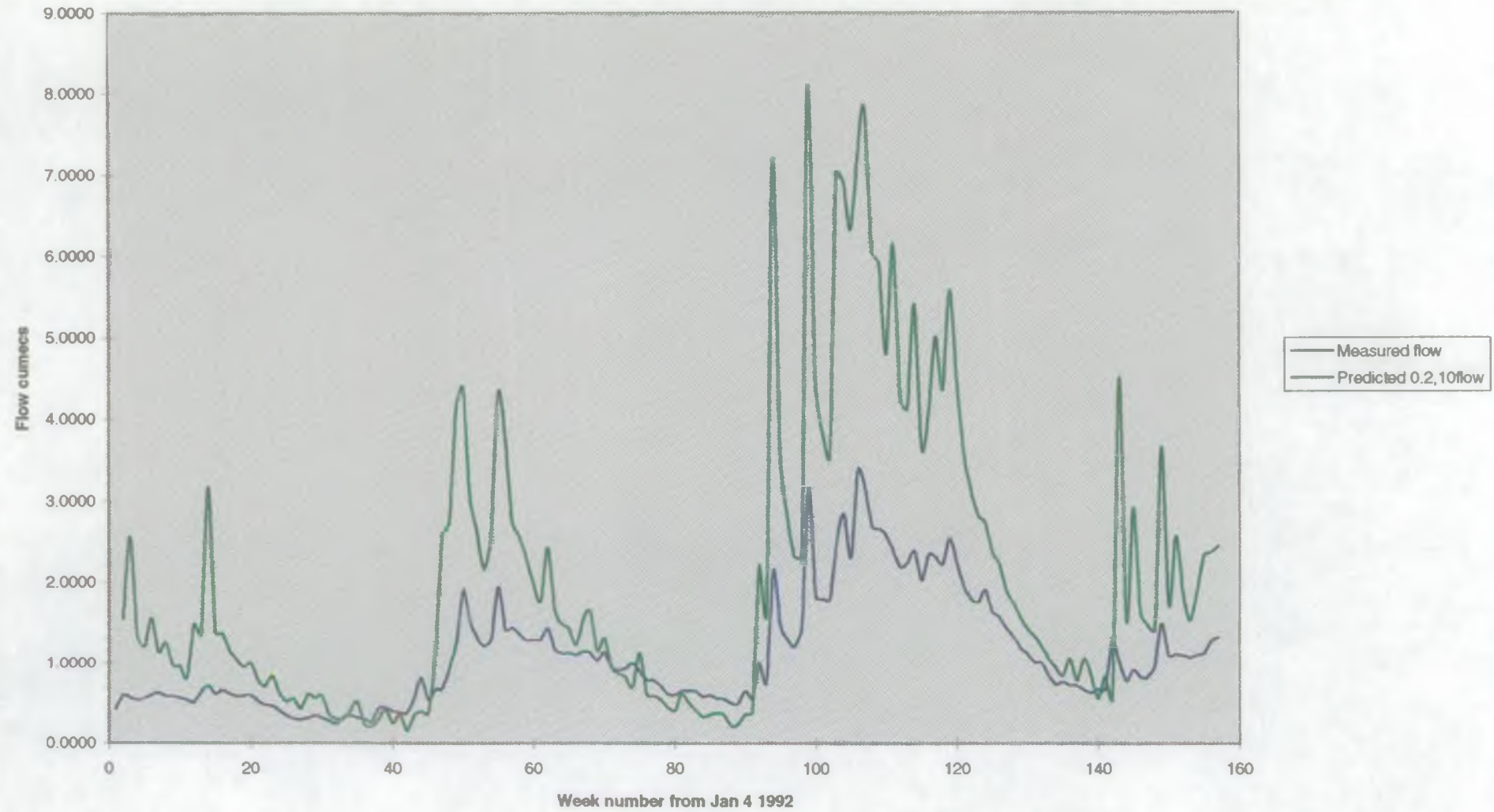
ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

RIVER WENSUM
034011

TG1648013240
TG1630013120
TG1622013230

NAR
033058

3007
TF7240012000

WENSUM

34011

34014

TG2100009700
TG2060009500

R. Nar weekly flows 1992-94

Legend:
- Measured flow
- Predicted 0.2,10flow

X-axis: Week number from Jan 4 1992

Y-axis: Flow cumecs

R. Nar Measured vs. Predicted flows

$y = 2.0291x$
$R^2 = 0.8239$

$y = 2.4121x - 0.5831$
$R^2 = 0.8543$

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

RIVER
CUCKMERE

041020

41016

41029

CUCKMERE

TQ5770007300

TQ5375008900

TQ532 0005050

TQ5320005050

41003
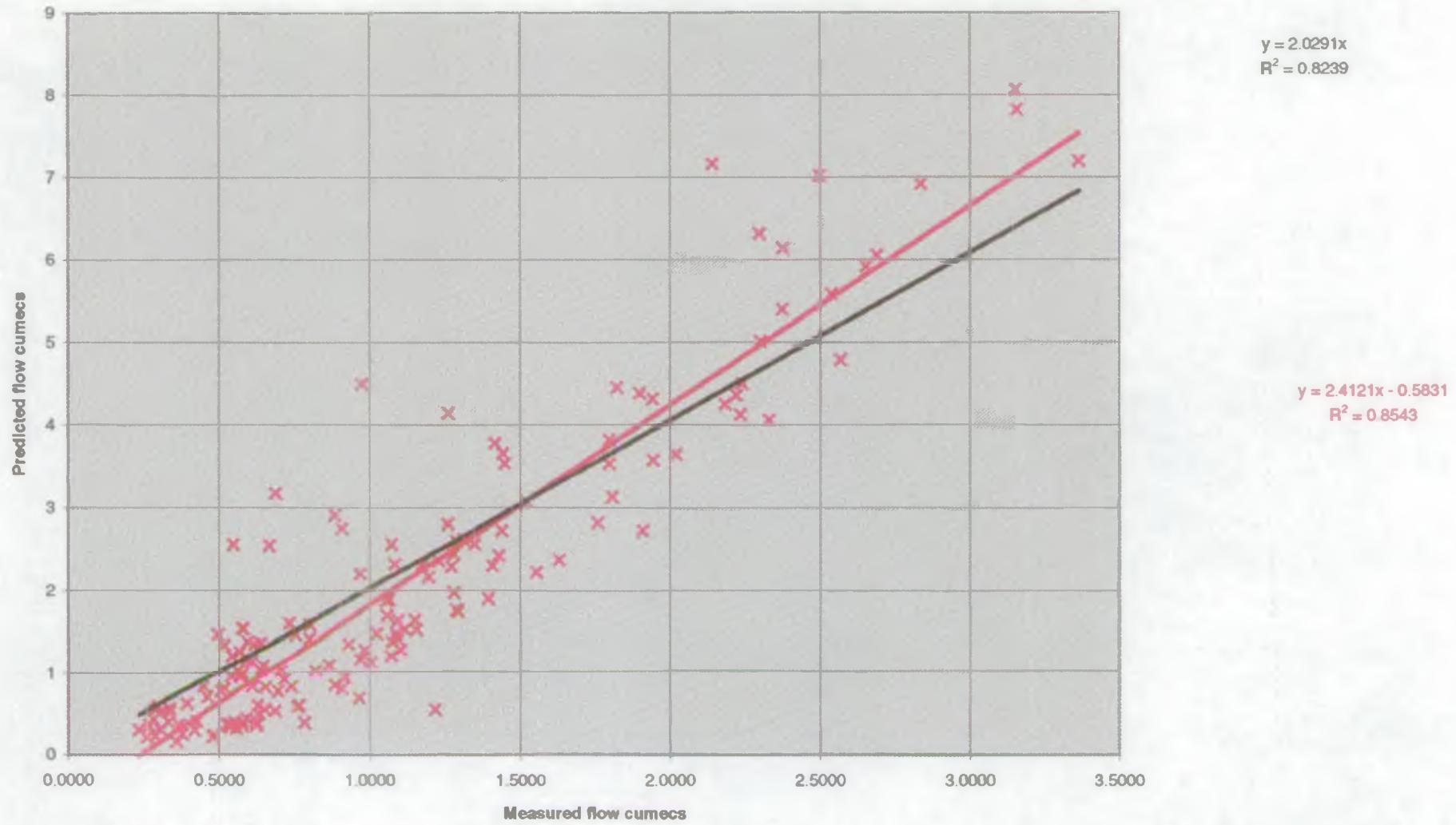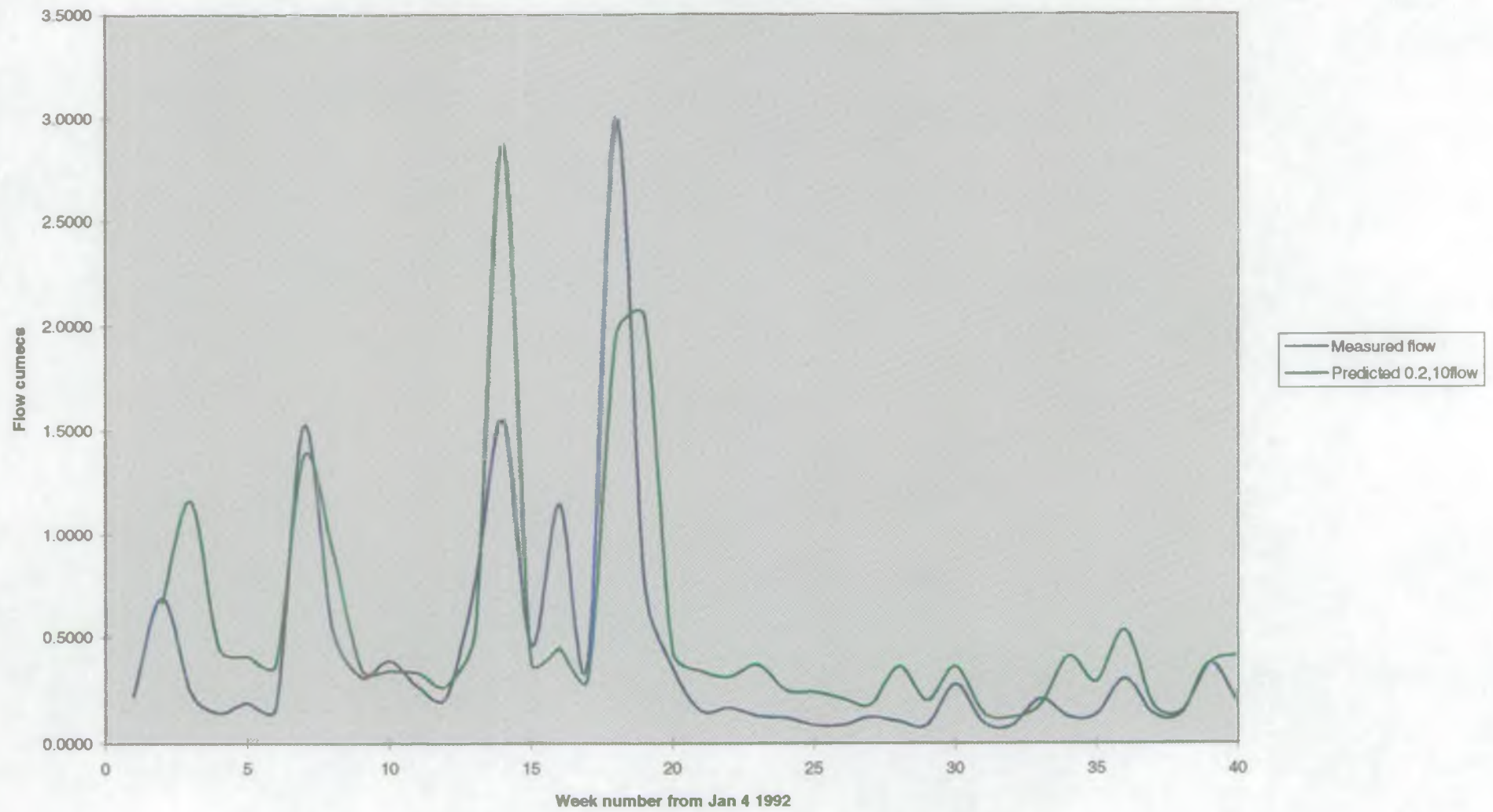
R. Cuckmere weekly flows 1992

R. Cuckmere weekly flows 1994
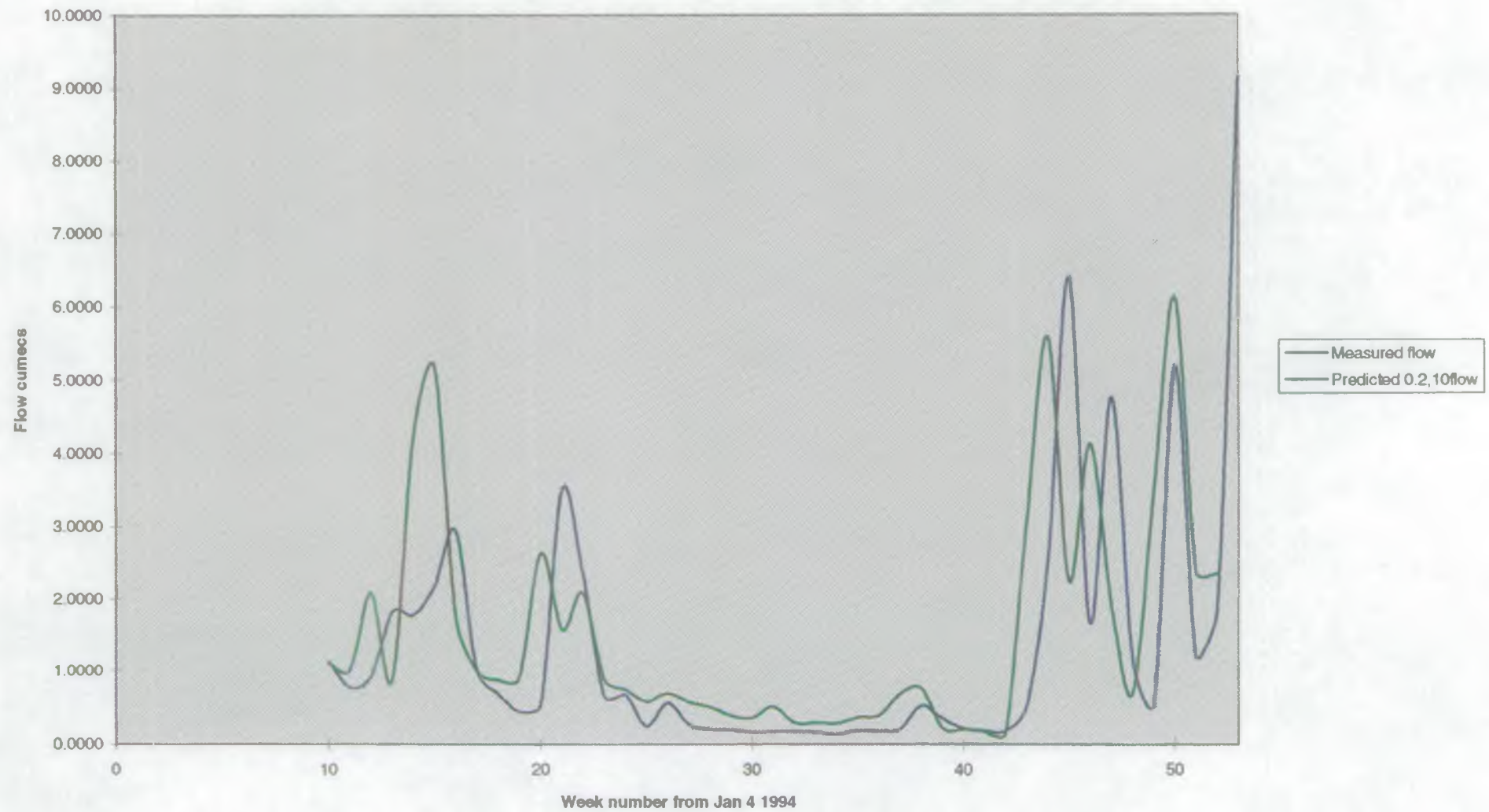
R. Cuckmere measured vs. predicted flows

$$y = 0.7053x + 0.4856$$
$$R^2 = 0.4181$$

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

ST2260013200

OTTER
045004B

OTTER

ST1680001200
ST1480000750

45008

SY0874088570

45005
SY0874088570

R. Otter weekly flows 1992-94

- Measured flow
- Predicted 0.2,10flow

Flow cumecs

Week number from Jan 4 1992
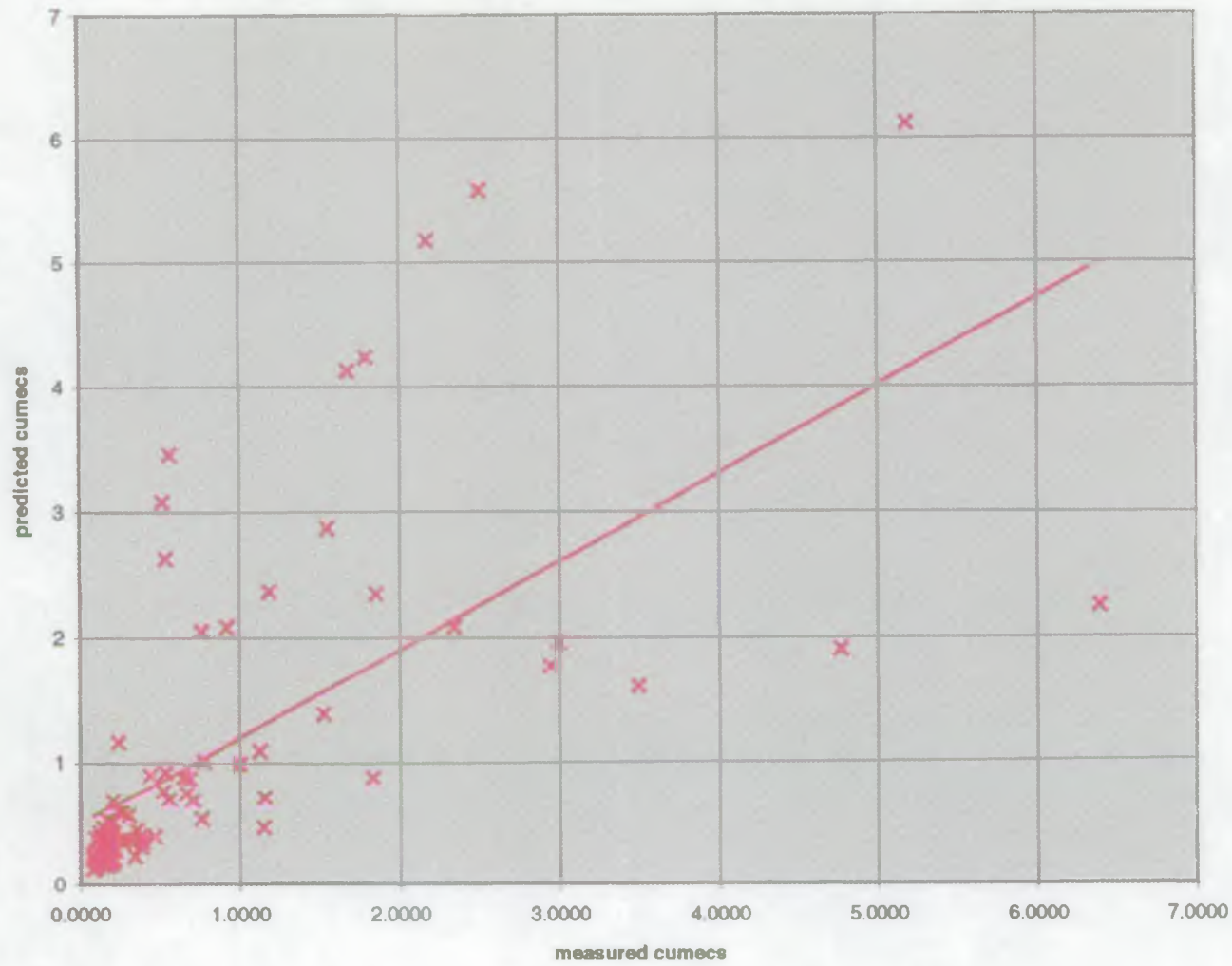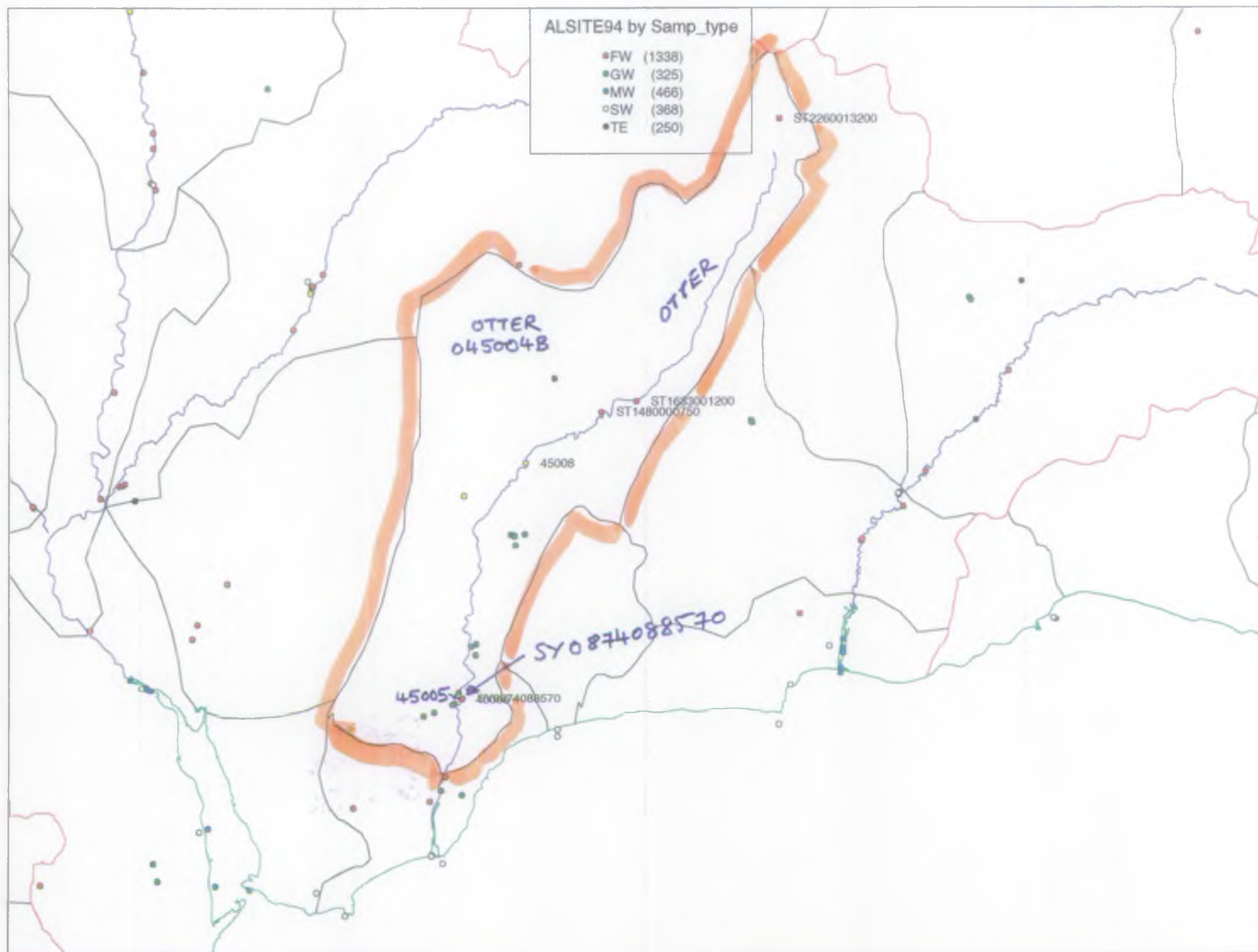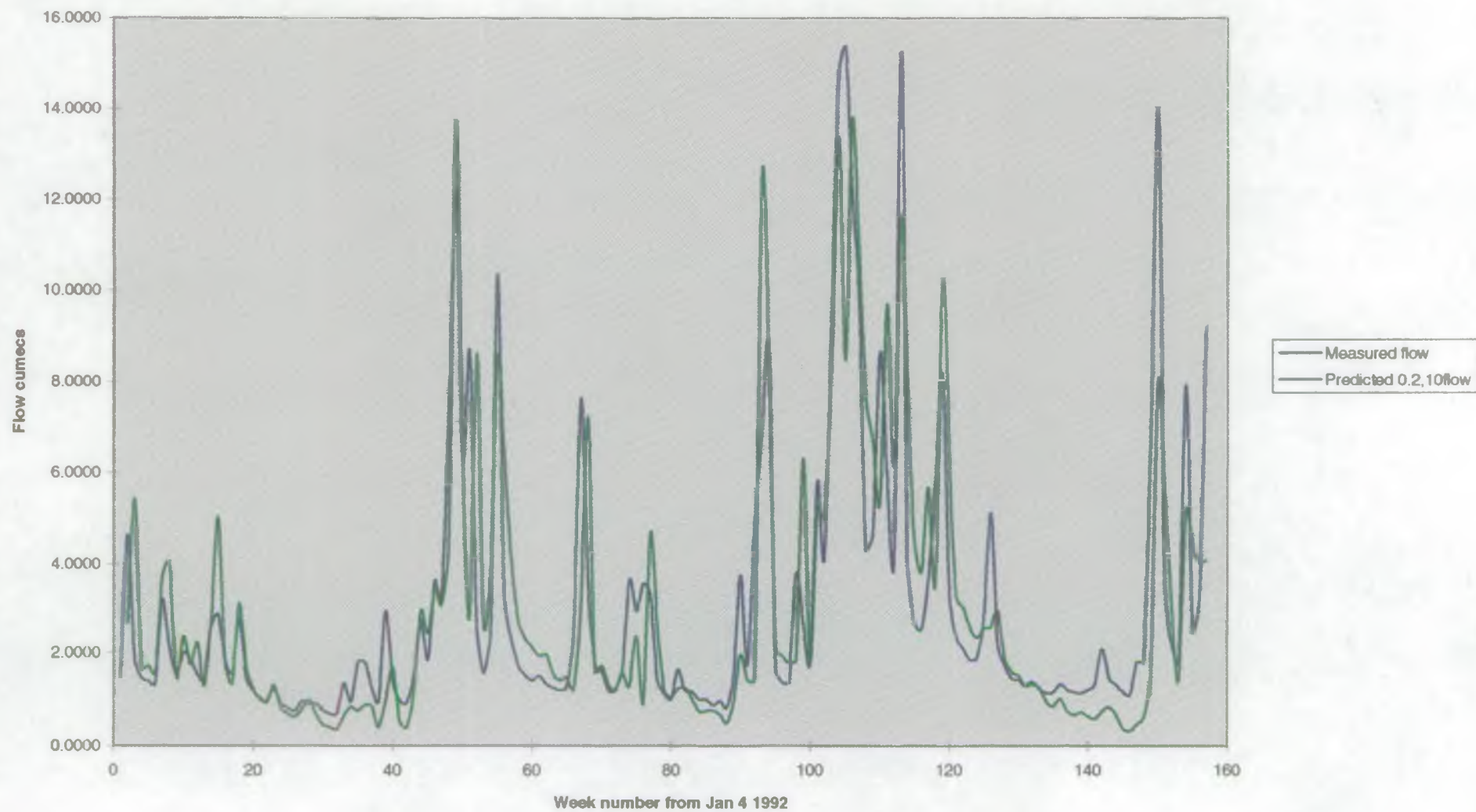
R. Otter measured vs. predicted flows

$y = 0.7883x + 0.589$
$R^2 = 0.6618$

predicted cumecs

measured cumecs

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

HAYLE
049022B

HAYLE

SW5490035560
SW5490035080
SW5495034900
49002

SW6145033070
SW6110032730
SW5961032410
SW6040032120
SW5661031960
SW5711031450
SW6362034862
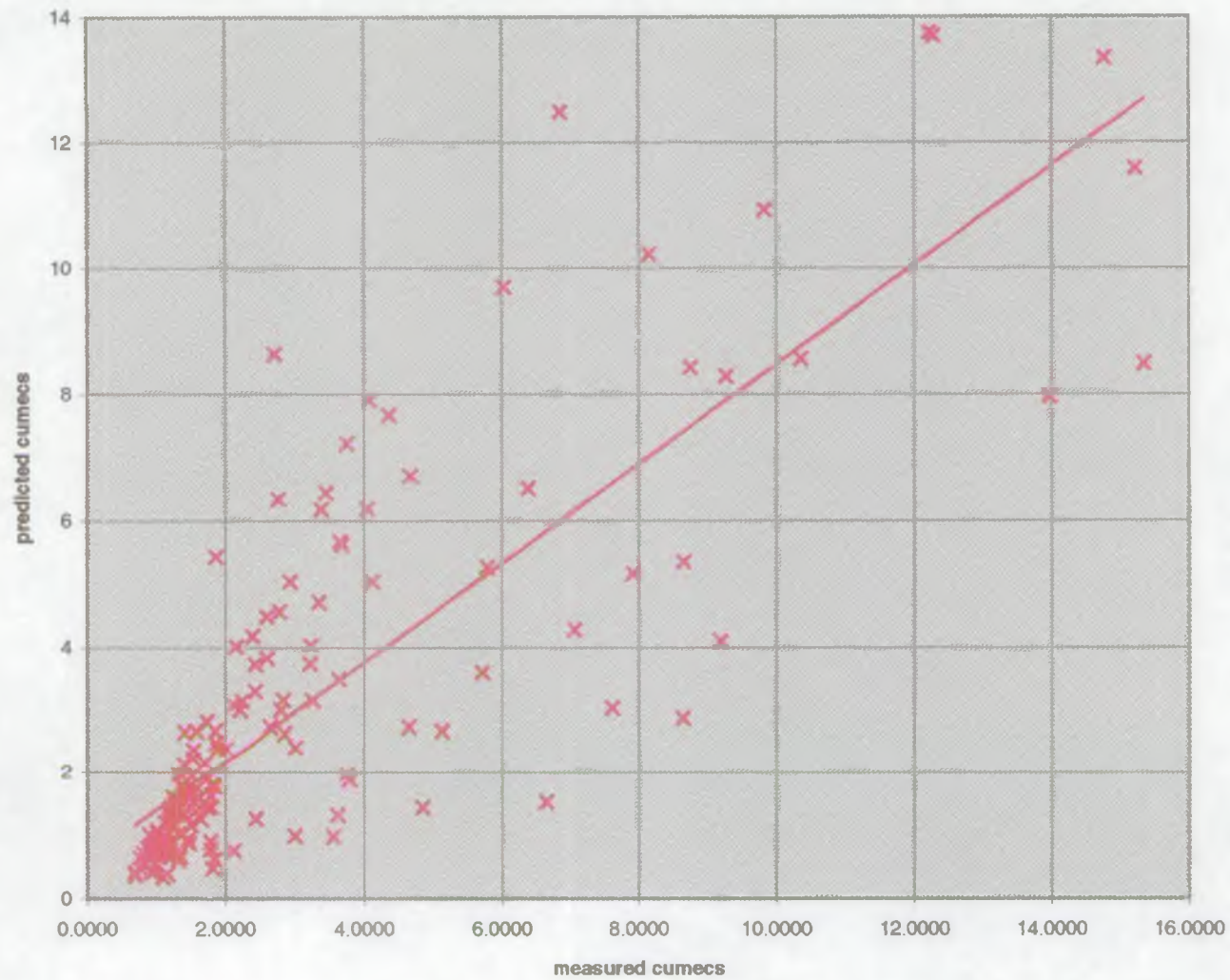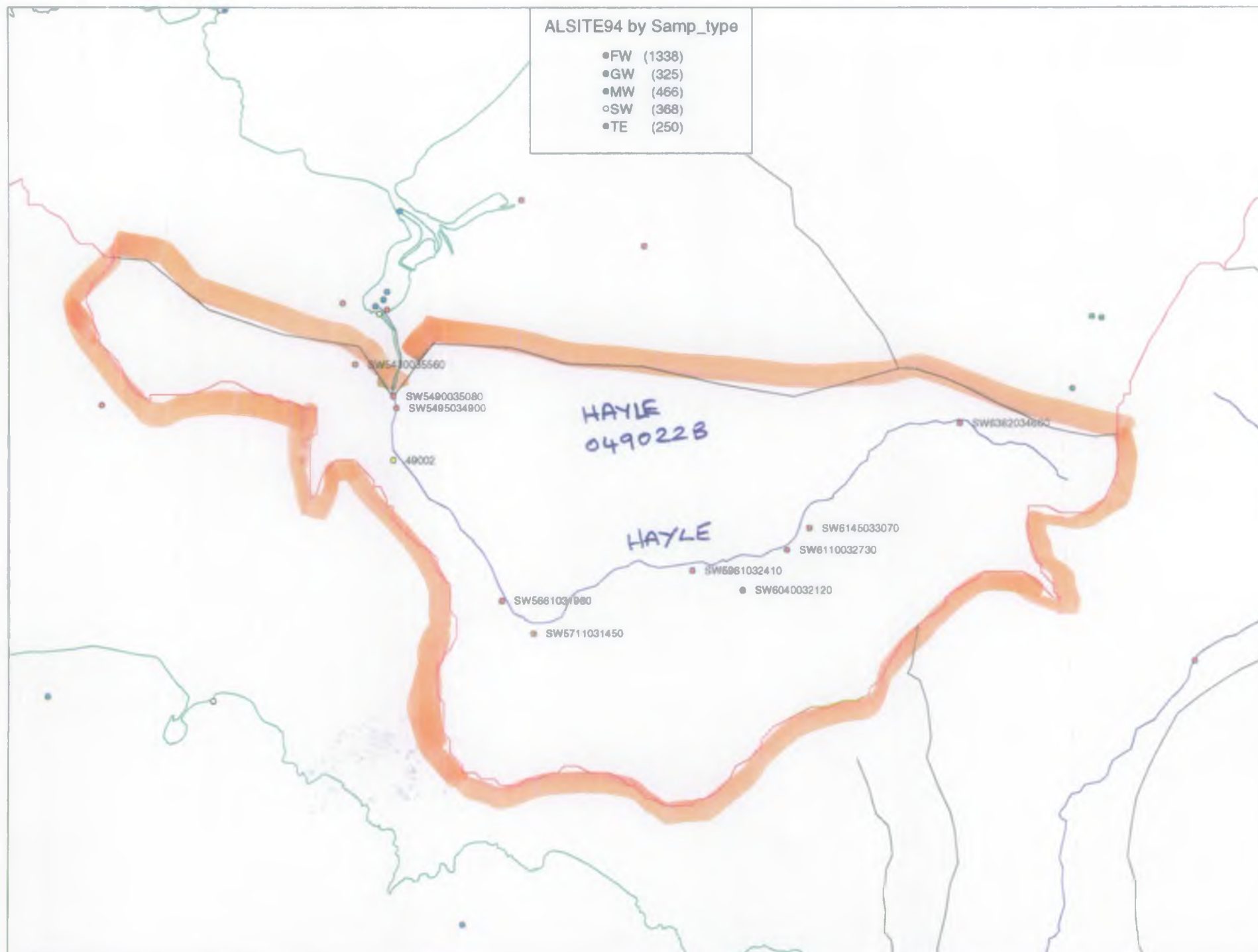
R. Hayle 1992-94 flows
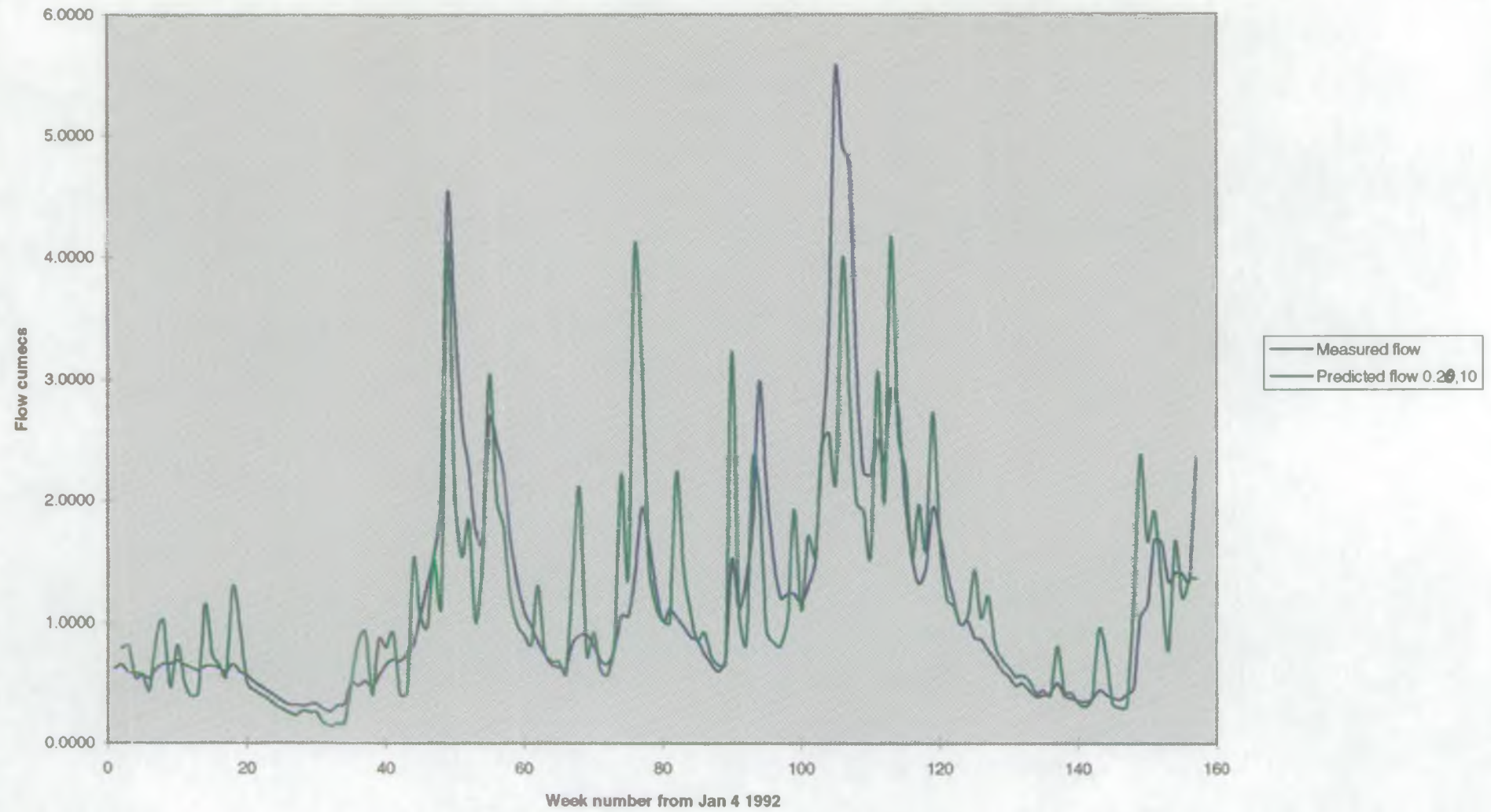
R. Hayle measured vs. predicted flows
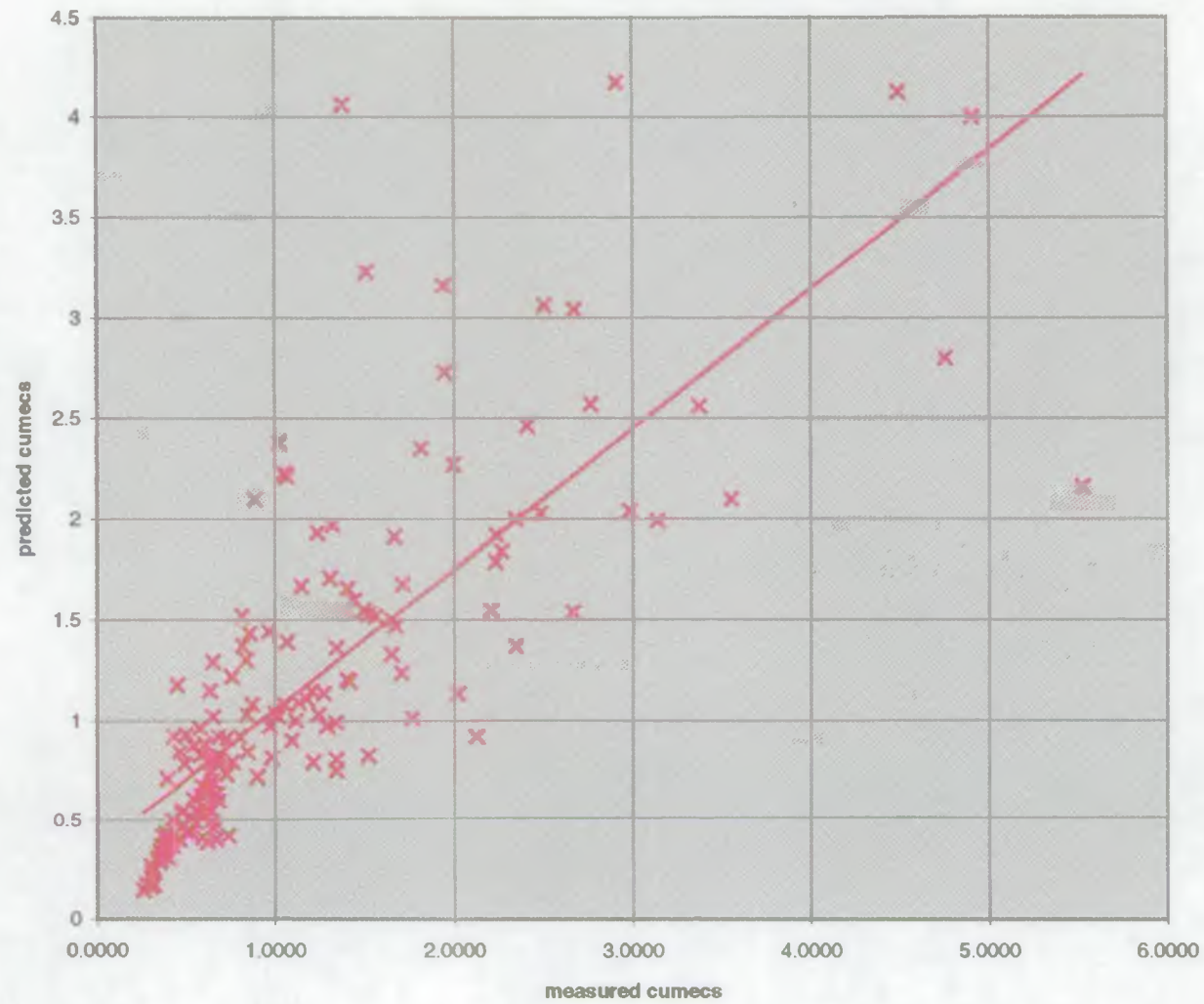
$y = 0.6956x + 0.3598$
$R^2 = 0.604$

TEST CATCHMENT 6

ALSITE94 by Samp_type
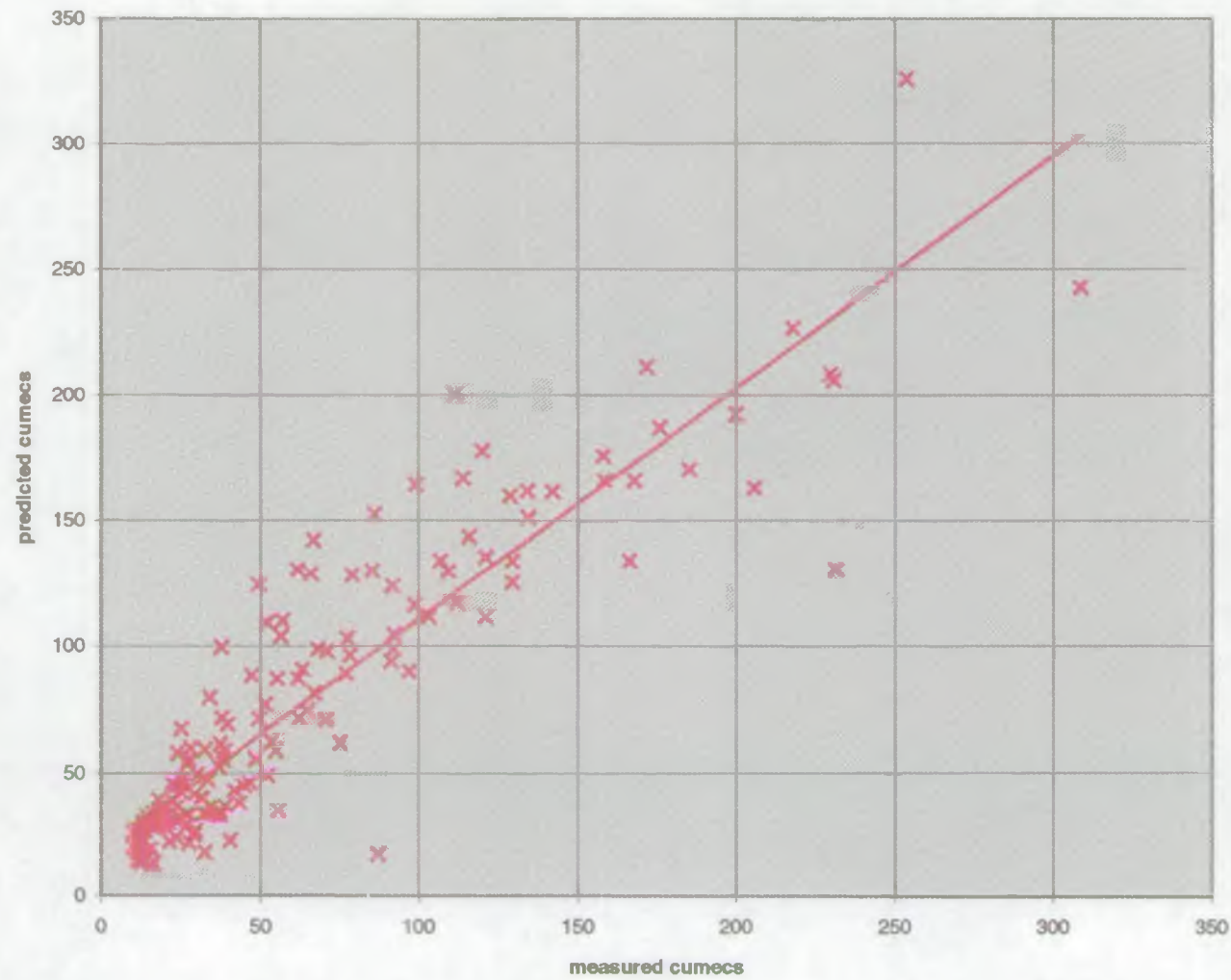
- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

RIVER PERRY 054003

RIVER RODEN 054004A

RIVER TERN 054004B

RIVER TERN 054004C

UPPER SEVERN RIVER TANAT 054001C

UPPER SEVERN (ABOVE MONTFORD) 054001A

UPPER MID SEVERN 054002A

RIVER TERN 054004D

UPPER SEVERN RIVER VYRNWY 054001E

UPPER SEVERN RIVER CAIN 054001D

UPPER SEVERN (ABOVE MONTFORD) 054001B

UPPER SEVERN R.TWRCH AND BANWY 054001F

UPPER MID SEVERN 054002B

UPPER MID SEVERN COUND BROOIE 054002C

RIVER WORFE 054005

UPPER SEVERN RIVER RHIW 054001G

UPPER SEVERN (ABOVE MONTFORD) 054001I

UPPER SEVERN (ABOVE MONTFORD) 054001J

UPPER SEVERN R.TRANNON, CLYWEDOG 054001H

UPPER MID SEVERN 054002D

R. Severn weekly flows 1992-94

Legend: Measured flow / Predicted 0.2,10flow

Y-axis: Flow cumecs

X-axis: Week number from Jan 4 1992
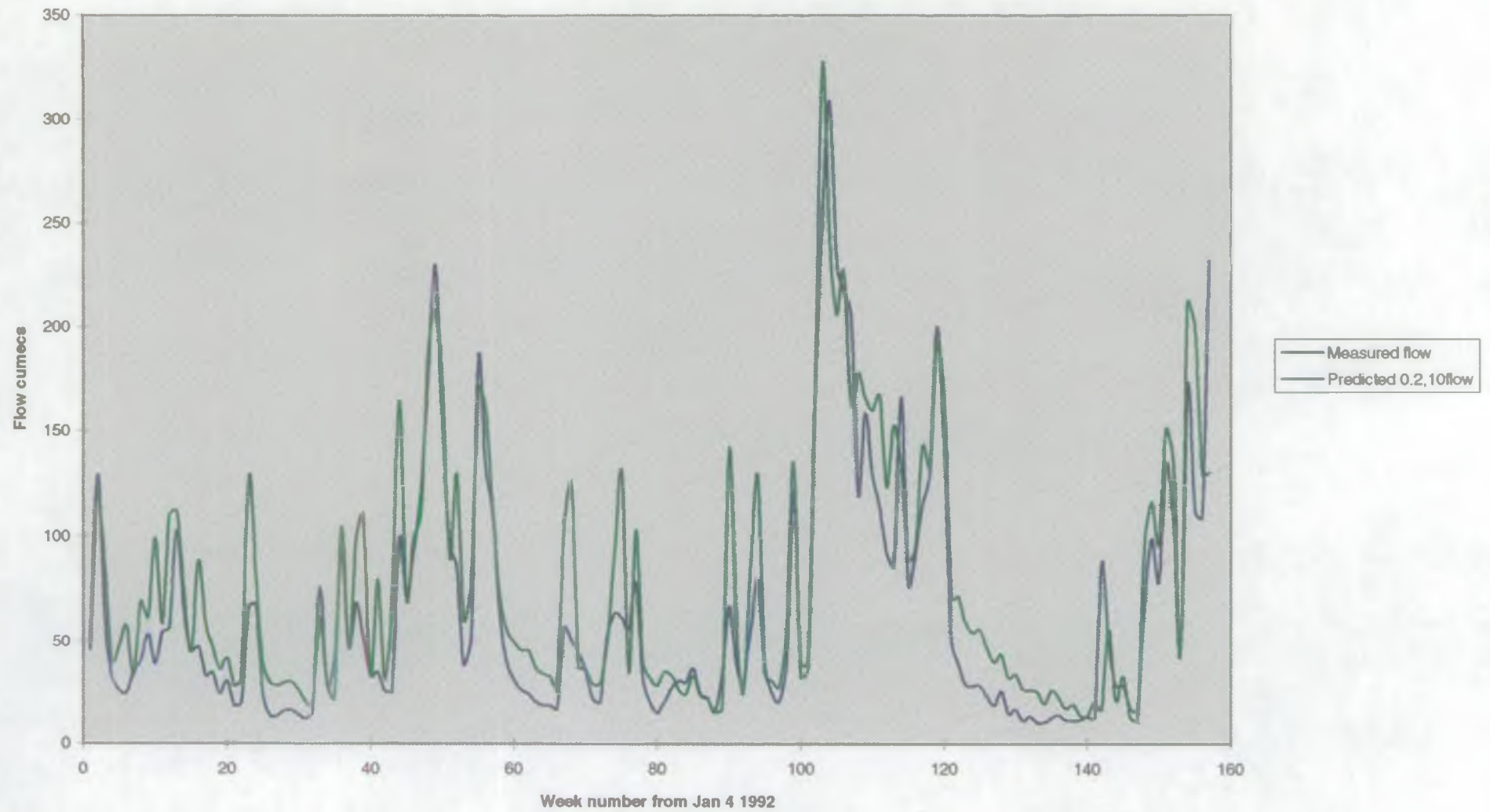
R. Severn measured vs. predicted flows

$y = 0.9227x + 18.302$
$R^2 = 0.8247$

TEST CATCHMENT 10

ALSITE94 by Samp_type

- FW (1338)
- GW (325)
- MW (466)
- SW (368)
- TE (250)

RIVER DOVE
034017

RIVER GIPPING
035008

10

35008

GIPPING

flow data.

TM050045100
TM190044800

GAUGING STATION
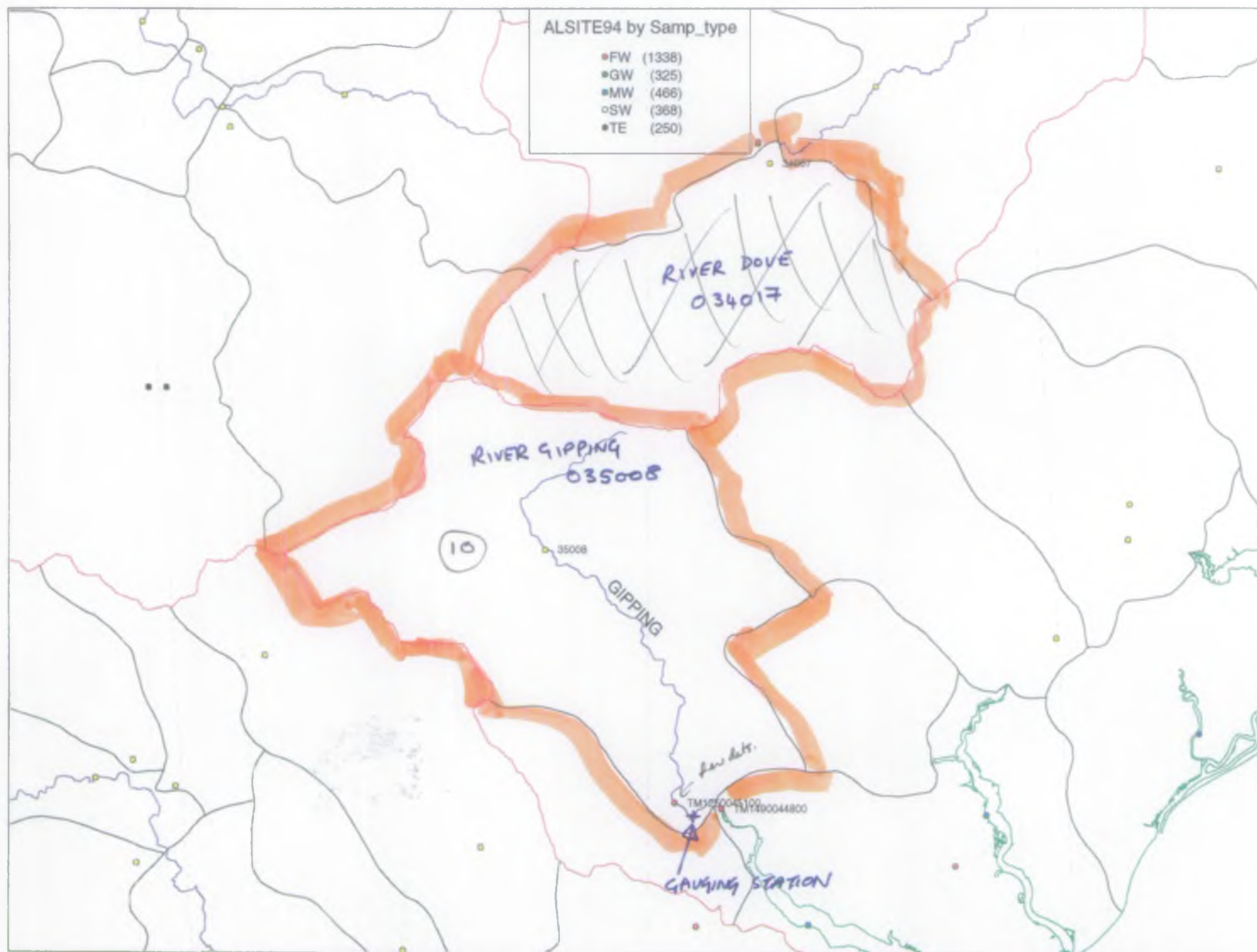
R. Gipping weekly flows 1992-94

Legend:
- Measured flow
- Predicted 0.2,10flow

Y-axis: Flow cumecs
X-axis: Week number from Jan 4 1992
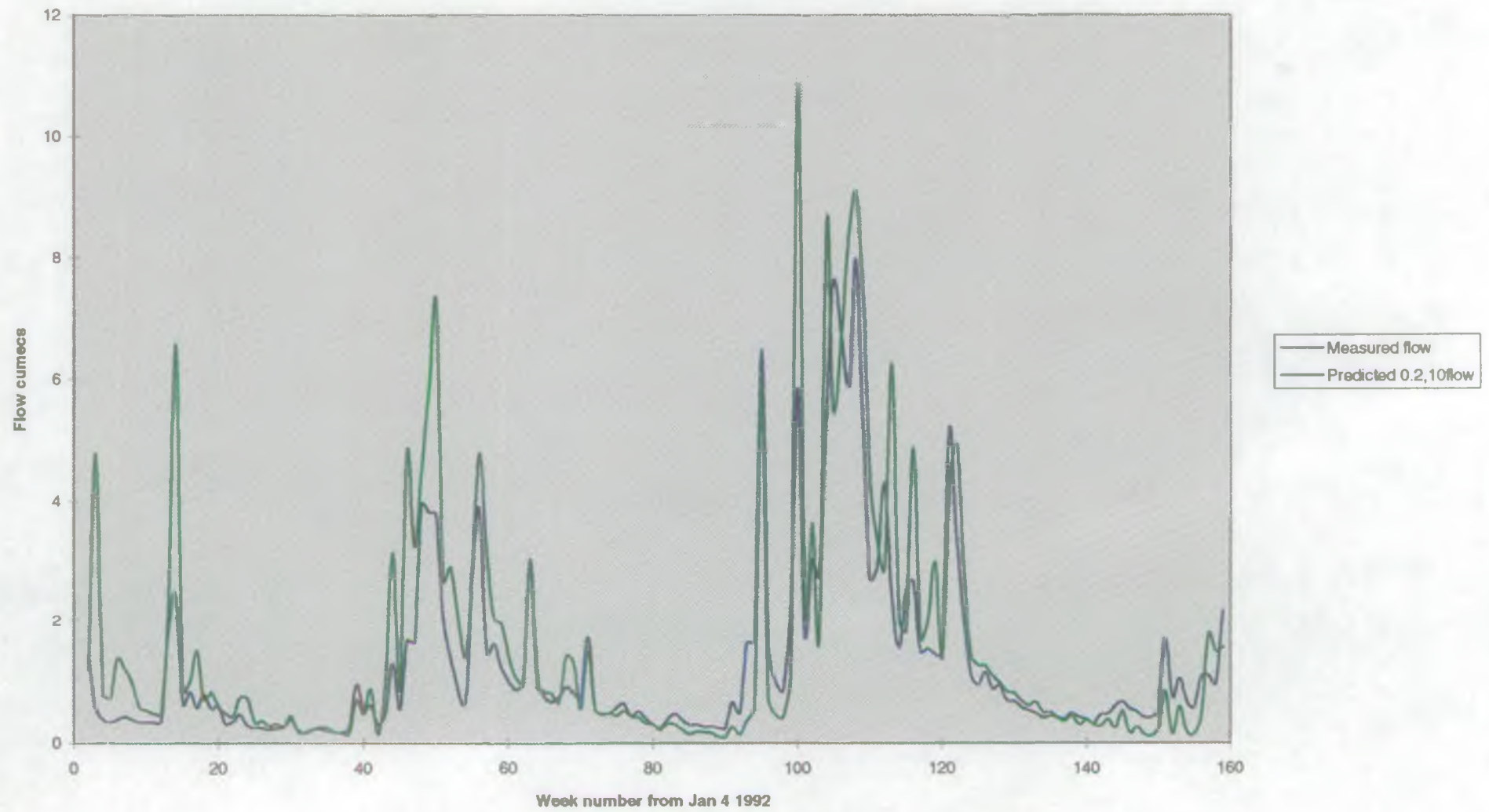
R. Gipping measured vs. predicted flows

$y = 1.207x + 0.0351$
$R^2 = 0.7709$
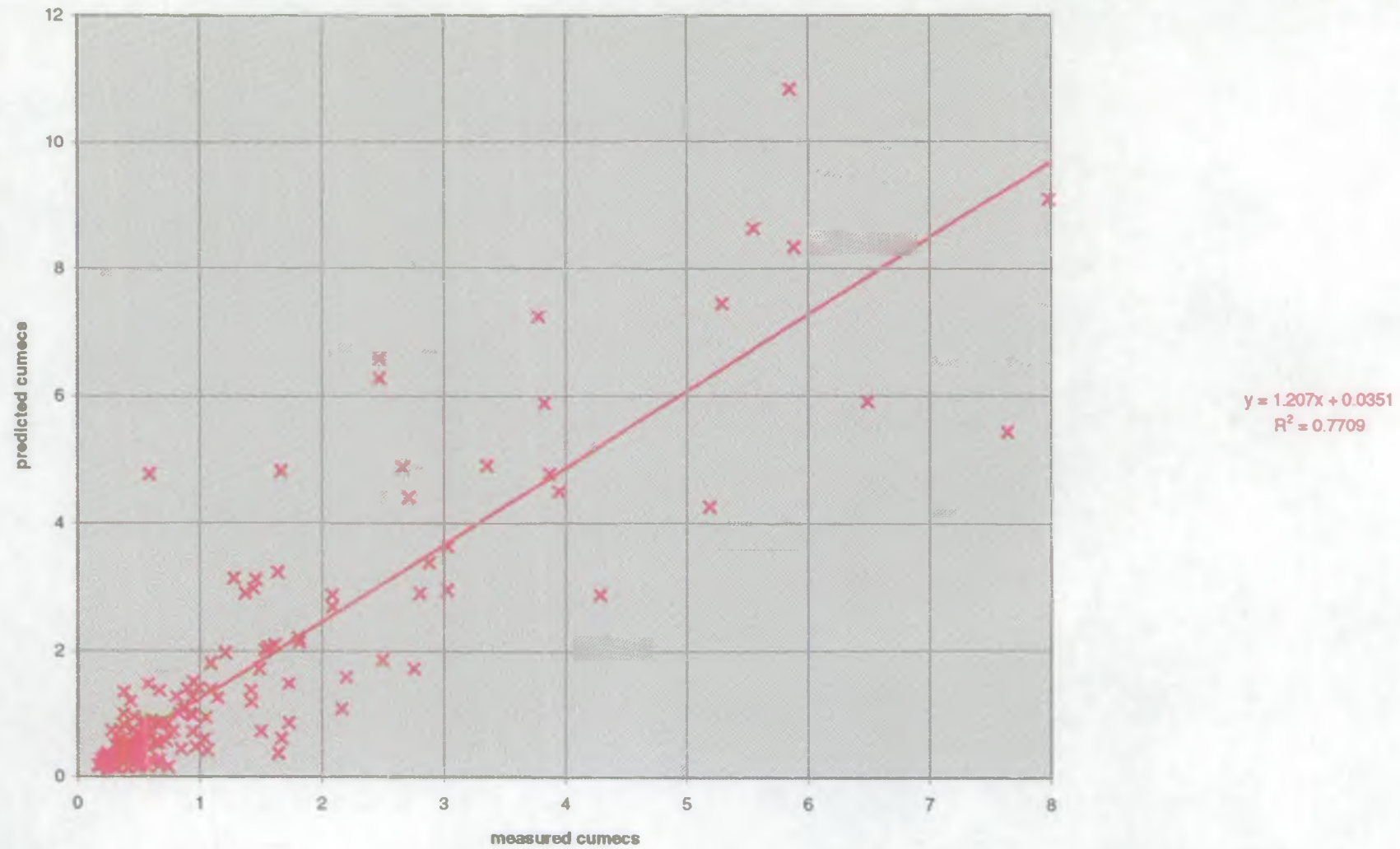
ANNEX III

COMPARISONS OF MEASURED AND SIMULATED PESTICIDE CONCENTRATIONS FOR TEST CATCHMENTS

Measured vs predicted concentrations for all test catchments and positive detections
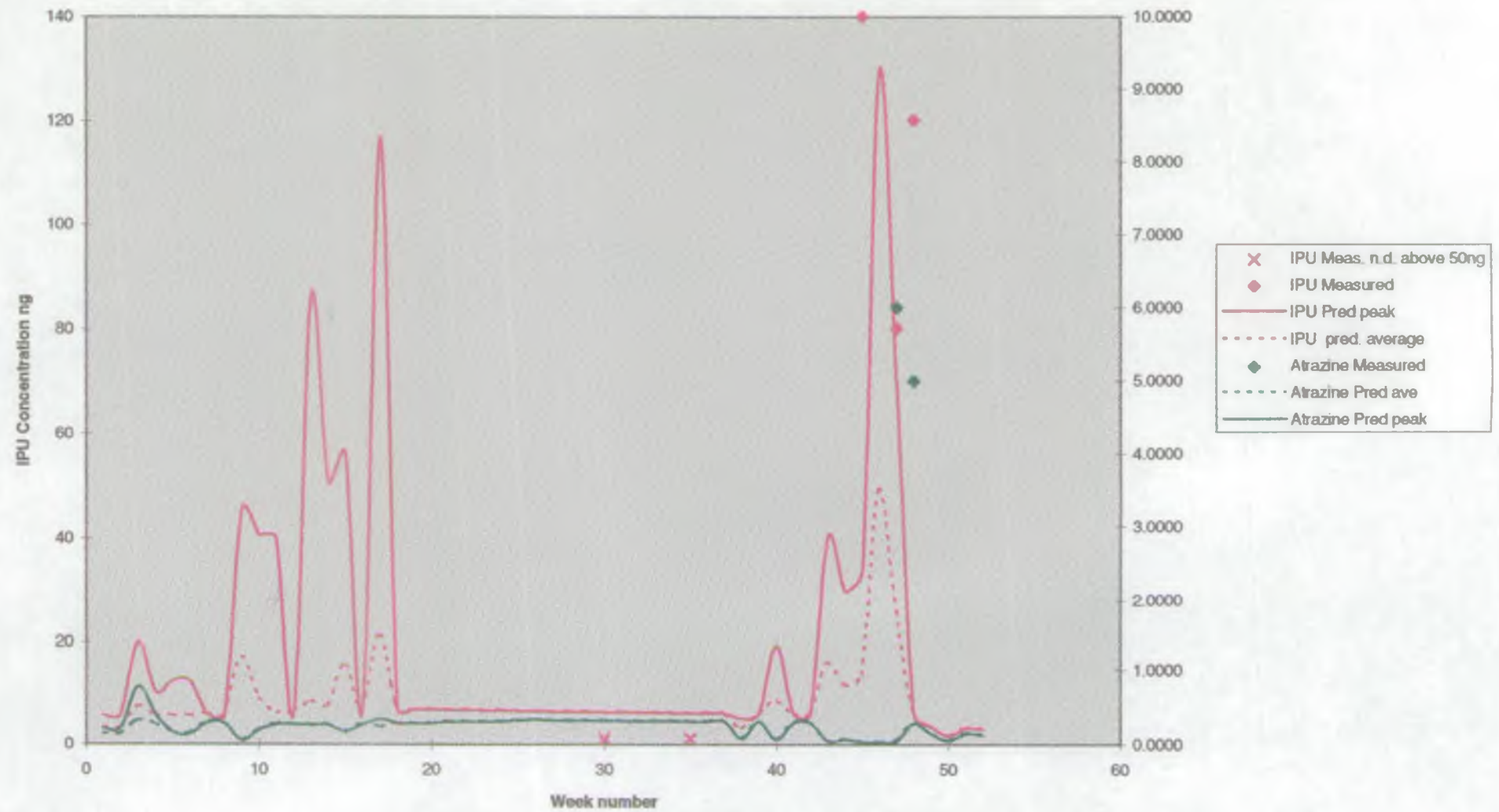

$y = 0.3063x$
$R^2 = 0.4076$
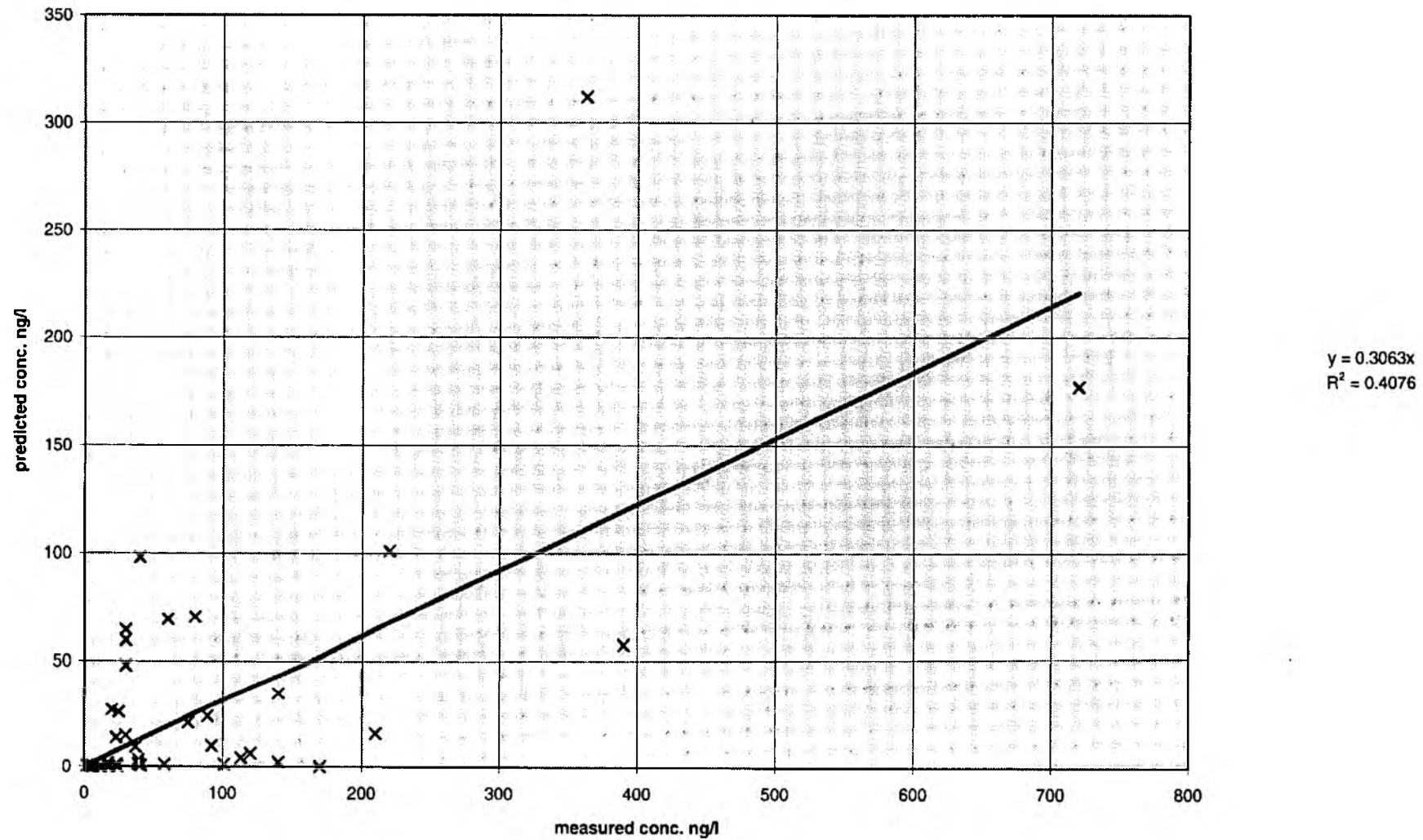
Measured vs Predicted concs for all pesticides in catchments excluding γHCH, atrazine, chlorfenvinphos & endosulfan

$y = 0.5436x$
$R^2 = 0.4623$
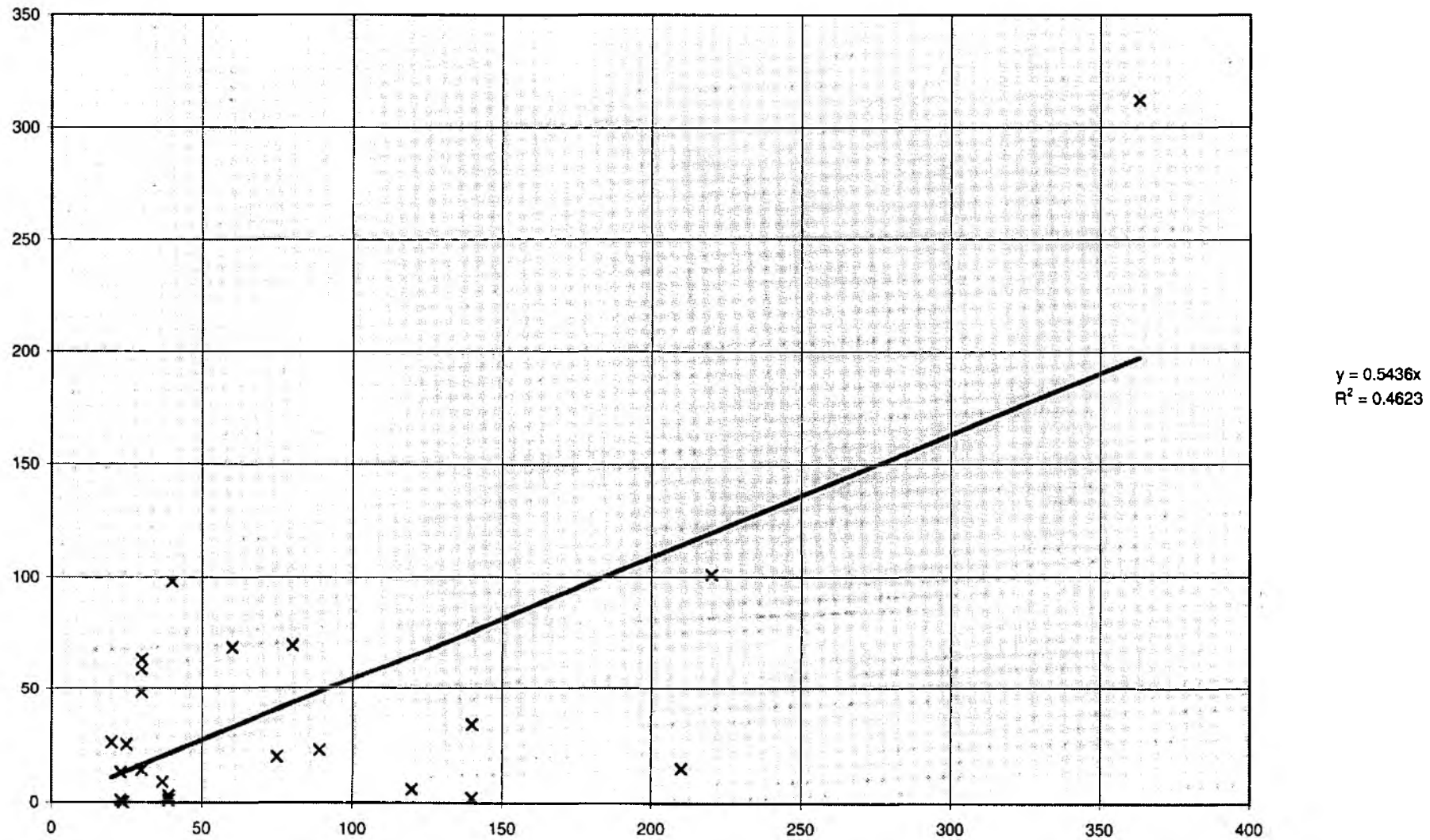
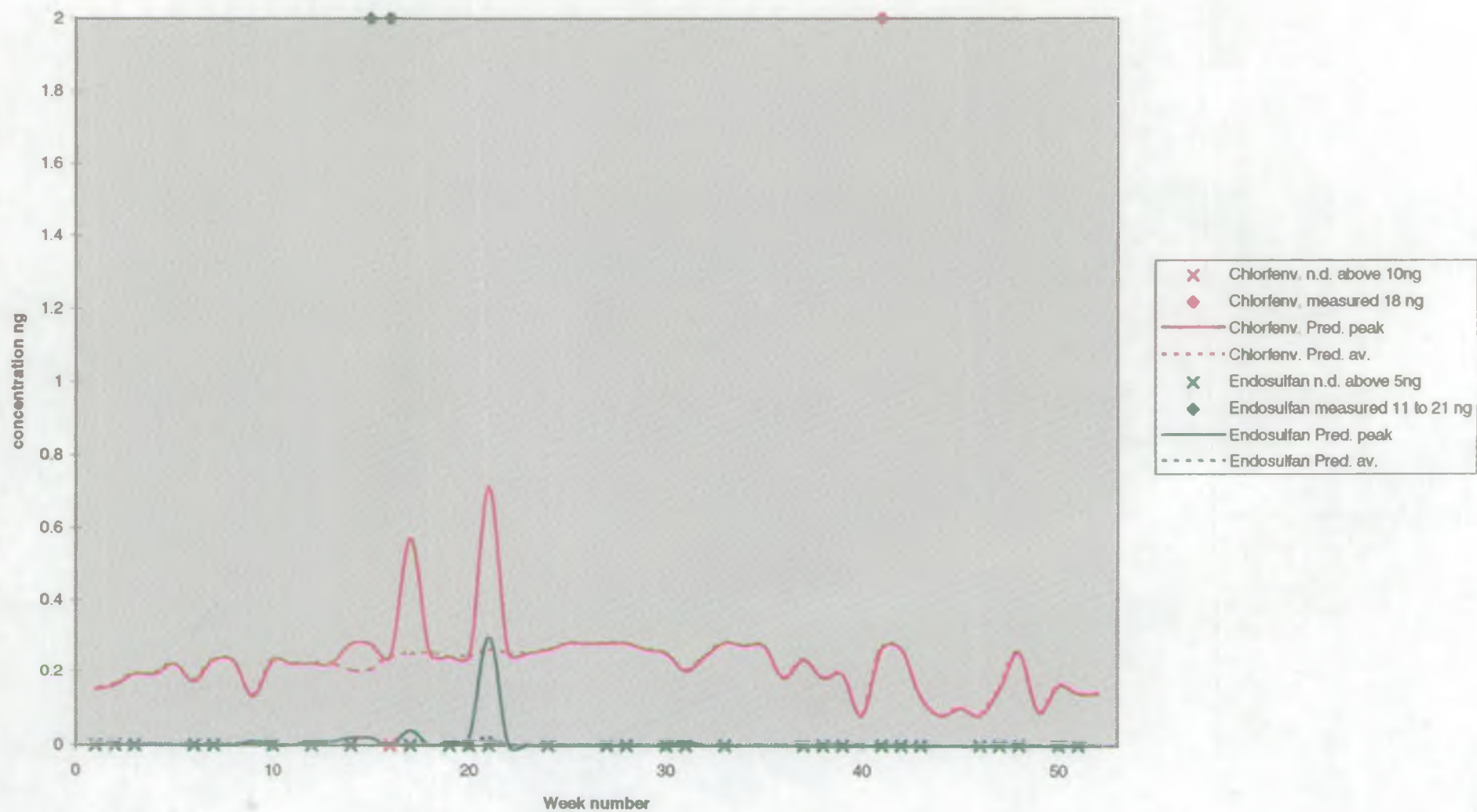## R. Wensum 1994 IPU & MCPA concs.
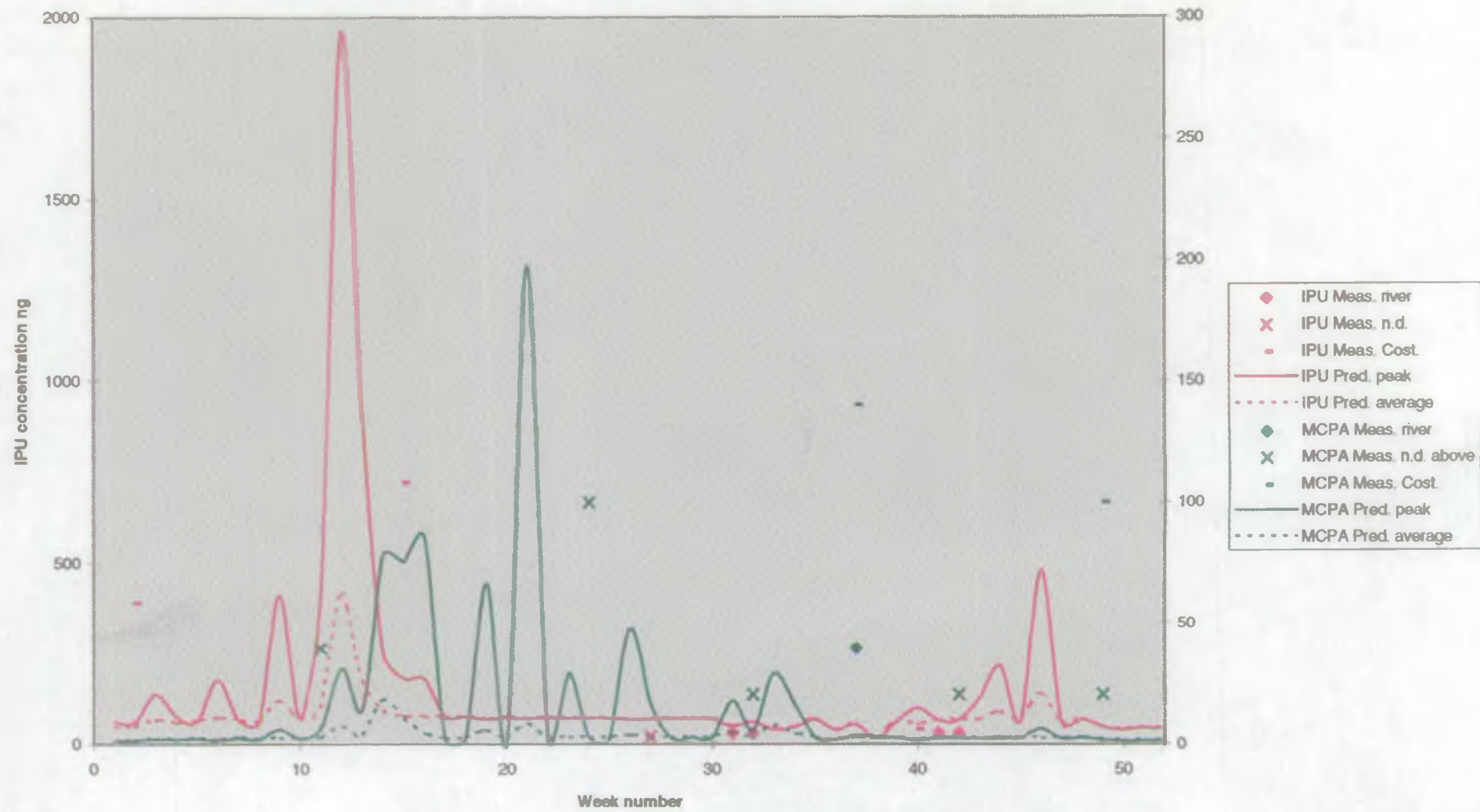
Master Chart 13

R. Coquet 1994 IPU and Atrazine concs.

R. Idle Chlorfenvinphos & Endosulfan concs., 1994

Legend:
- × Chlorfenv. n.d. above 10ng
- ◆ Chlorfenv. measured 18 ng
- —— Chlorfenv. Pred. peak
- ····· Chlorfenv. Pred. av.
- × Endosulfan n.d. above 5ng
- ◆ Endosulfan measured 11 to 21 ng
- —— Endosulfan Pred. peak
- ····· Endosulfan Pred. av.

Y-axis: concentration ng

X-axis: Week number

R. Teifi 1994 mecoprop and IPU concs.

Legend:
- ✗ mecoprop n.d. above 100 ng
- ◆ mecoprop measured
- —— mecoprop pred. peak
- - - - mecoprop pred. av.
- ◇ IPU n.d. above 100
- —— IPU pred. peak
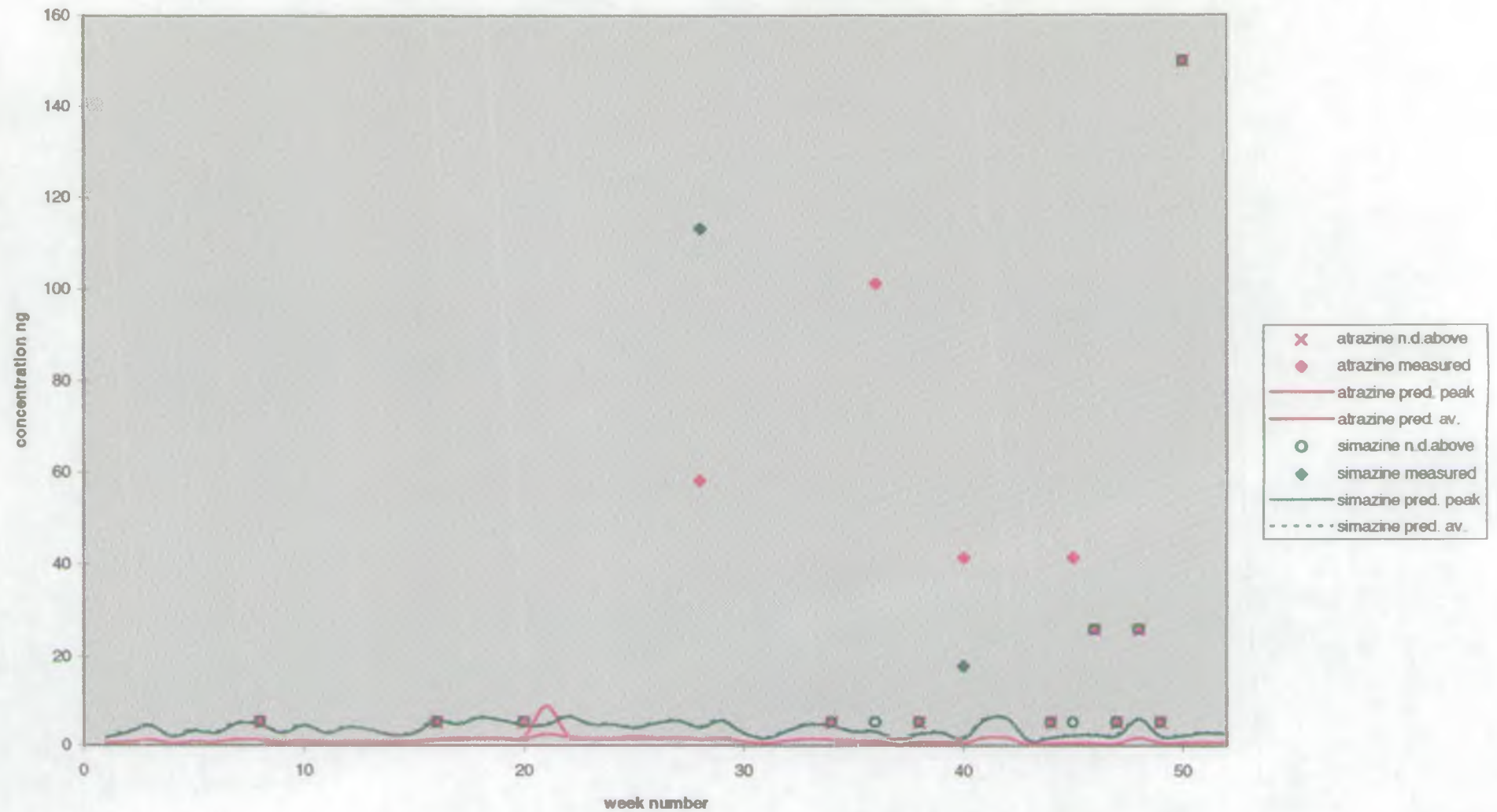- - - - IPU pred. av.

Concentration ng (y-axis)
Week number (x-axis)
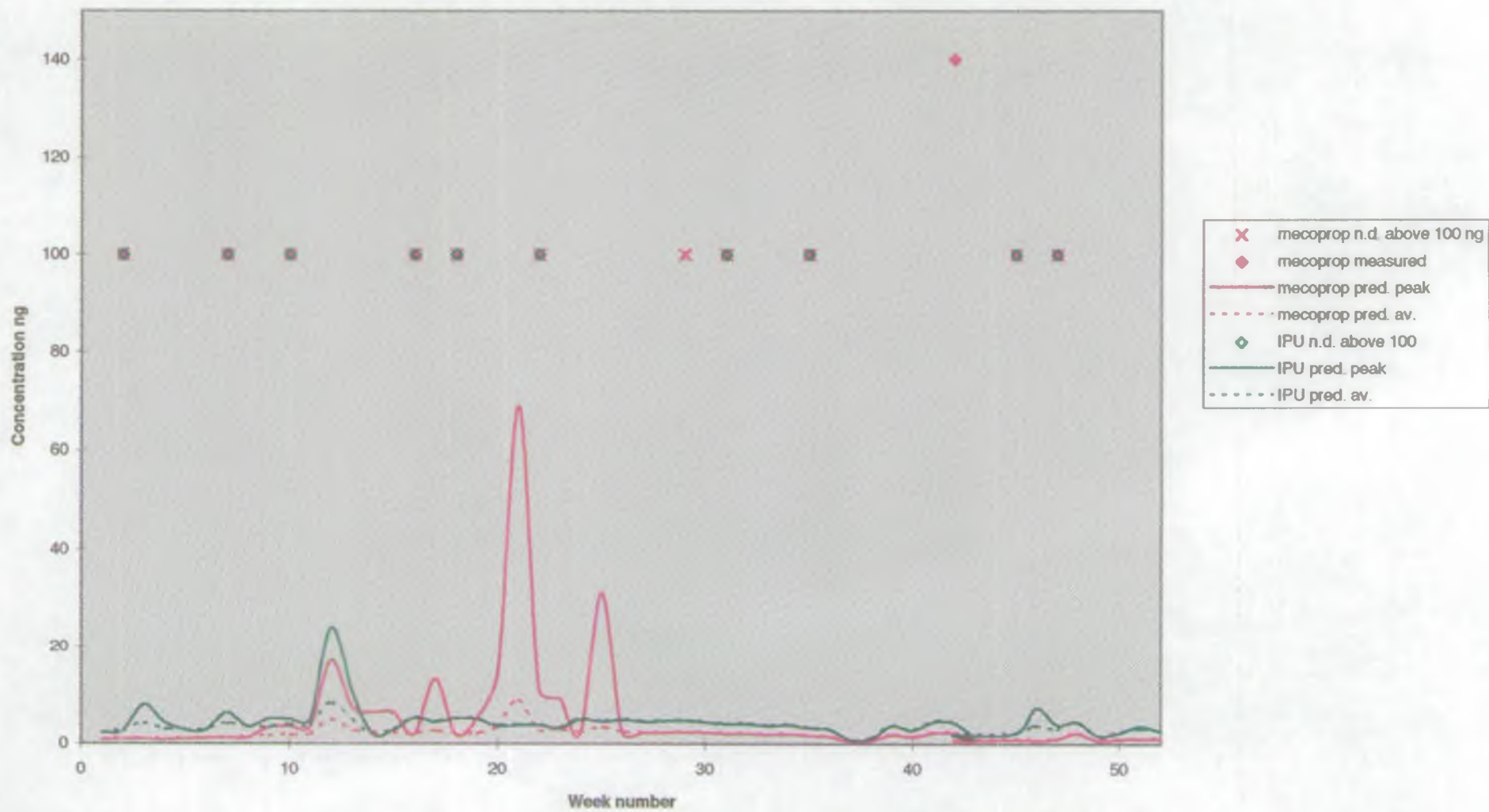
R. Teifi 1994 gamma HCH and Simazine concs.
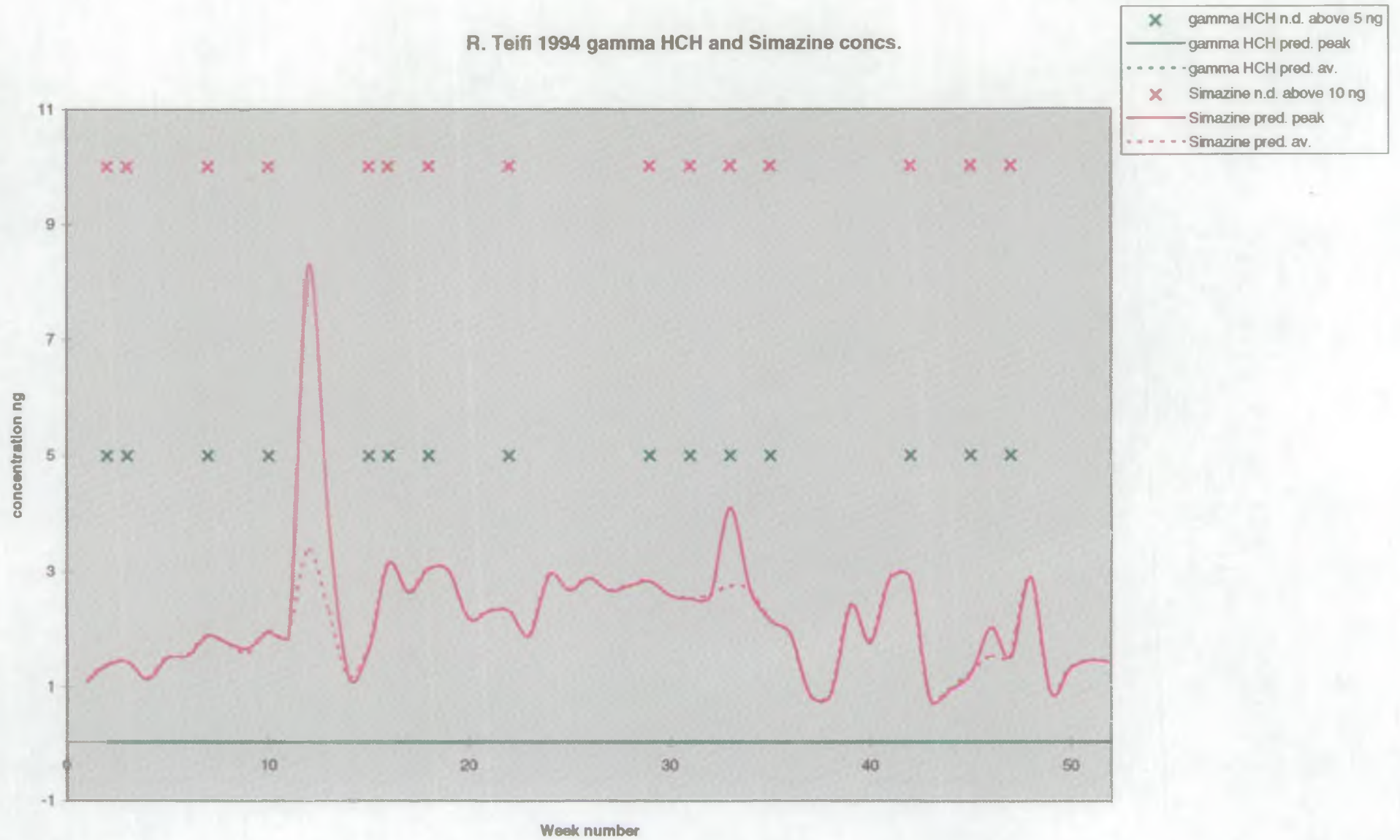
R. Darwen 1994 atrazine & simazine concs.

R. Darwen 1994 chlorvenfinphos & fenitrothion concs.

R. Nene 1994 IPU & mecoprop concs.
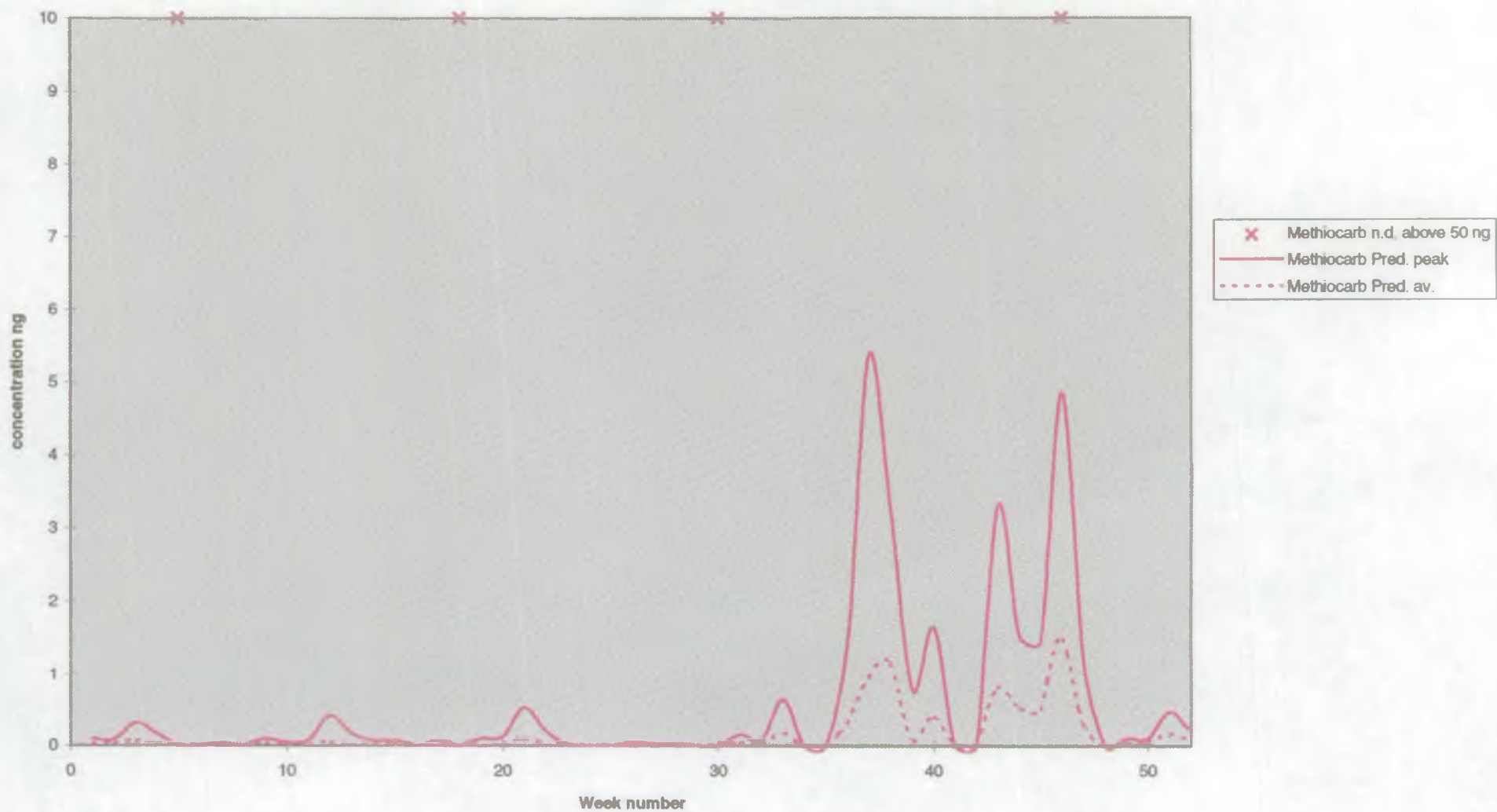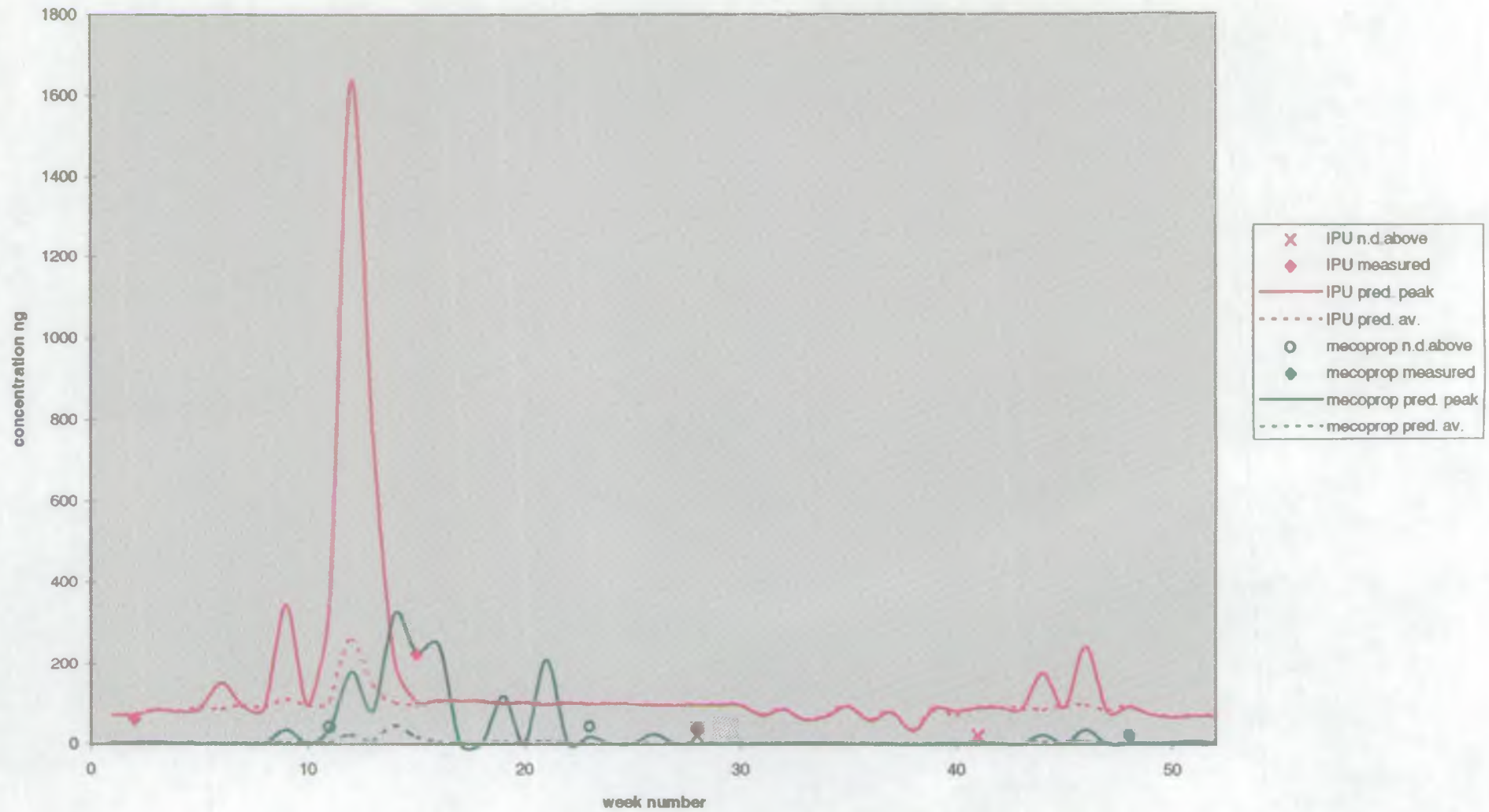

Legend:
- ◆ IPU Measured conc. 5720
- ■ IPU Measured conc. 34800
- ▲ IPU Measured
- ── IPU pred. peak
- ····· IPU Pred. av.
- ✕ Mecoprop n.d. above 40 ng
- ▲ Mecoprop measured
- ── Mecoprop Pred. peak
- ····· Mecoprop Pred. av.

X-axis: Week number
Y-axis: concentration ng
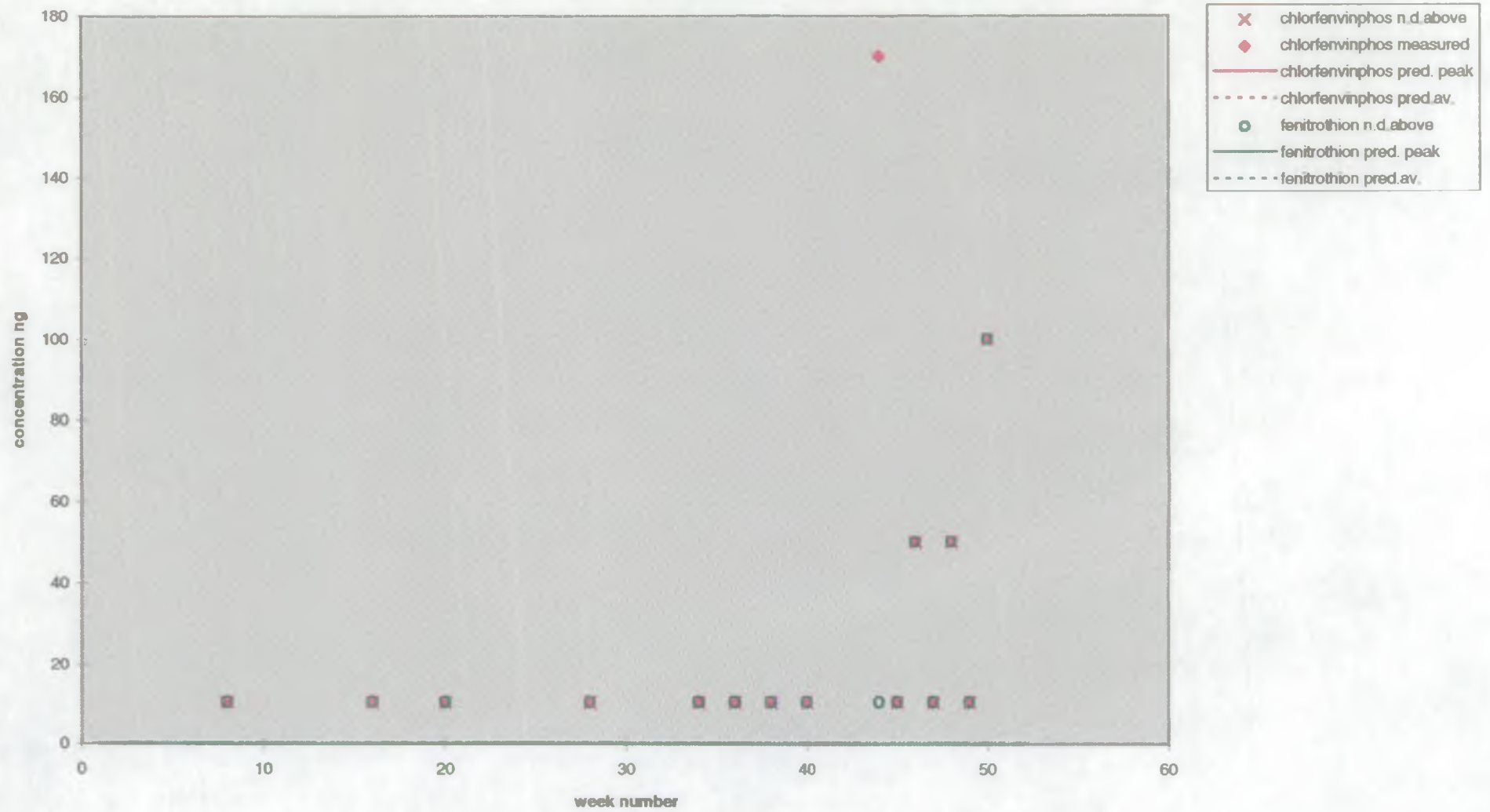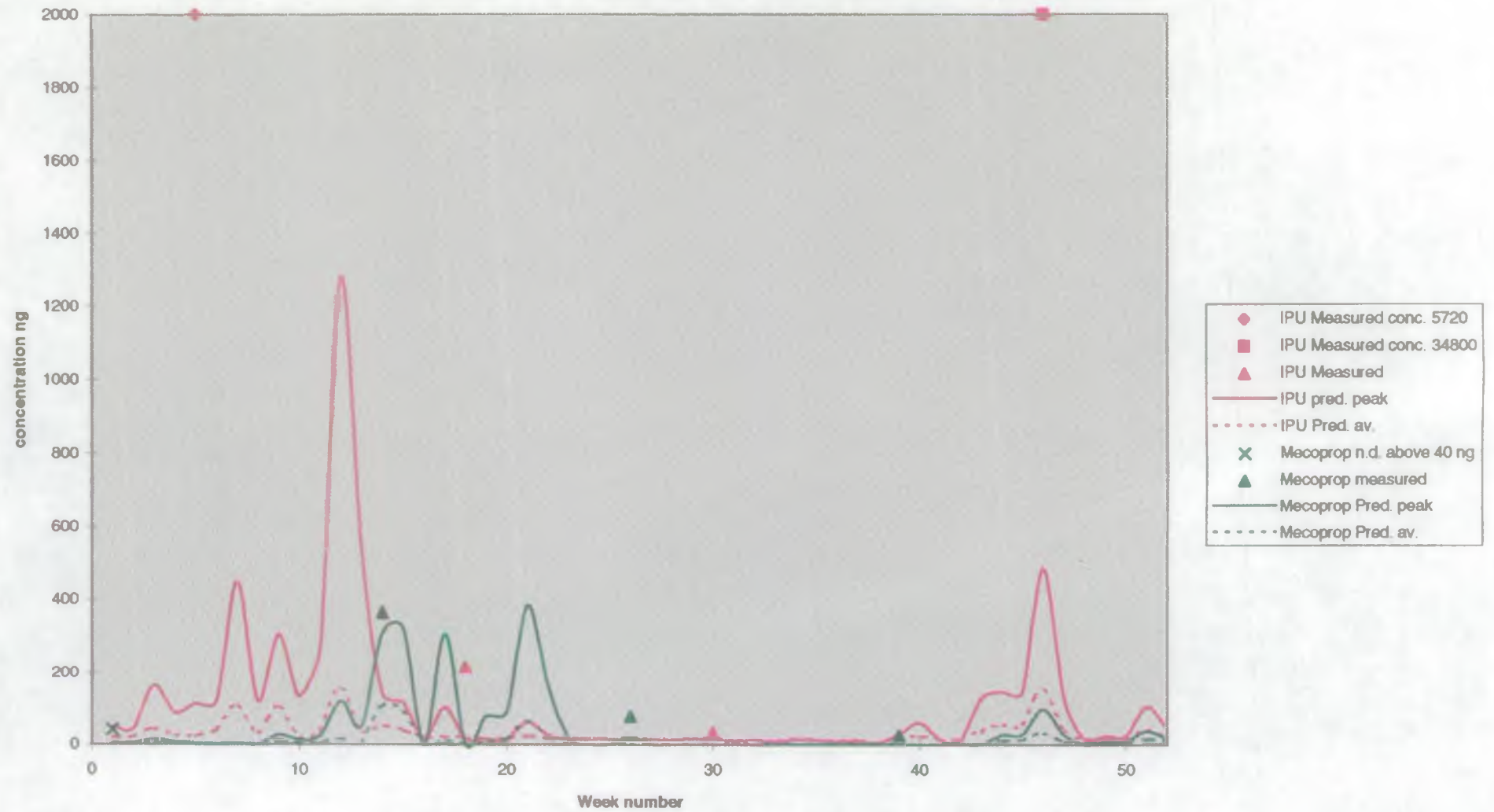
R. Nene 1994 methiocarb concs

R.Nar 1994 IPU & mecoprop concs.

Legend:
- X   IPU n.d.above
- ◆   IPU measured
- —   IPU pred. peak
- - - -   IPU pred. av.
- O   mecoprop n.d.above
- ◆   mecoprop measured
- —   mecoprop pred. peak
- - - -   mecoprop pred. av.

x-axis: week number
y-axis: concentration ng

R. Nar 1994 trietazine & methiocarb concs.
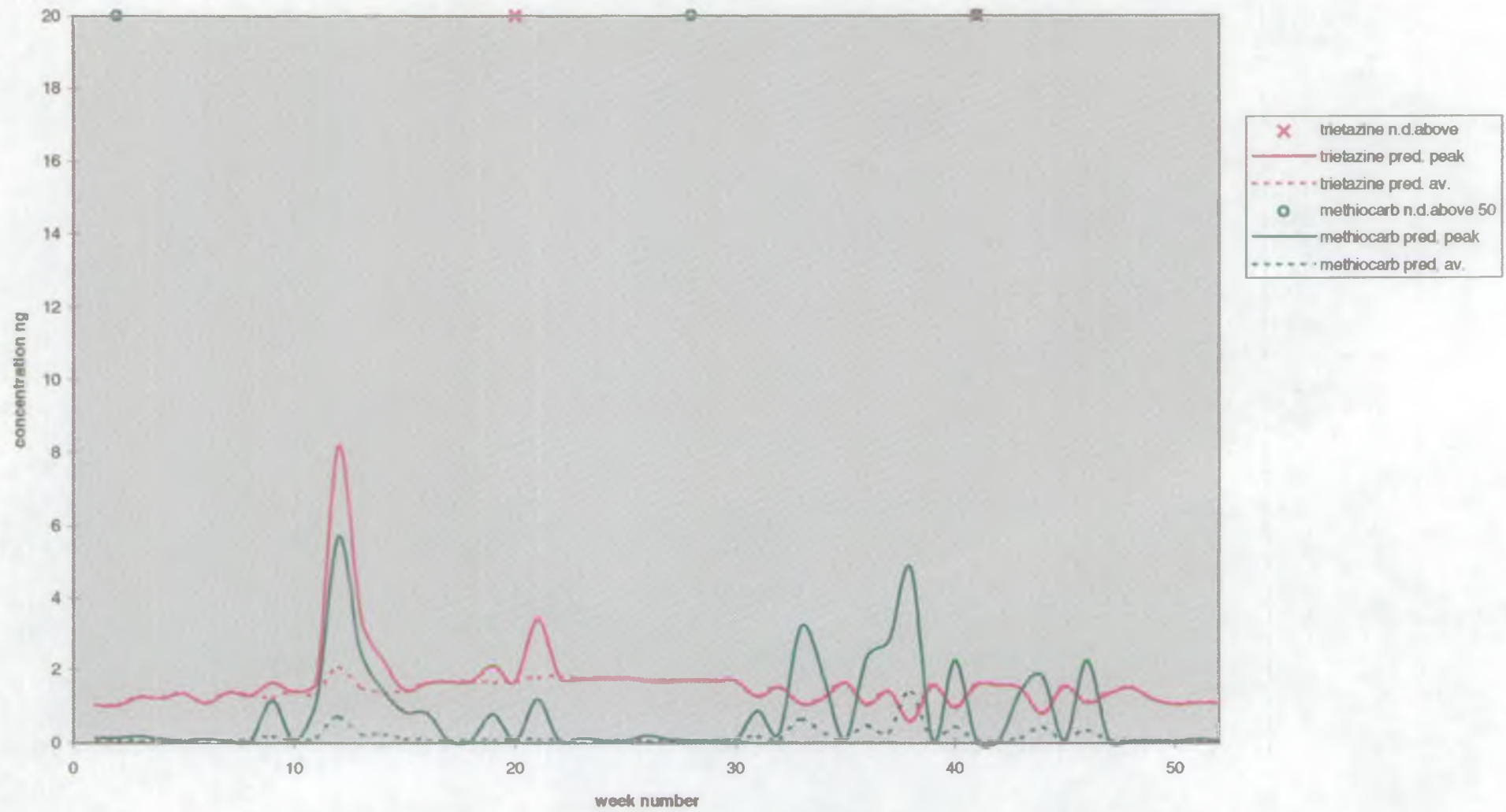
R. Cuckmere 1994 Fenitrothion & Simazine concs.

Legend:
- × simazine n.d. above
- ◆ simazine measured
- —— simazine pred. peak
- ····· simazine pred. av.
- ○ fenitrothion n.d. above
- —— fenitrothion pred. peak
- ····· fenitrothion pred. av.

Axis labels: concentration ng (y-axis), Week number (x-axis)
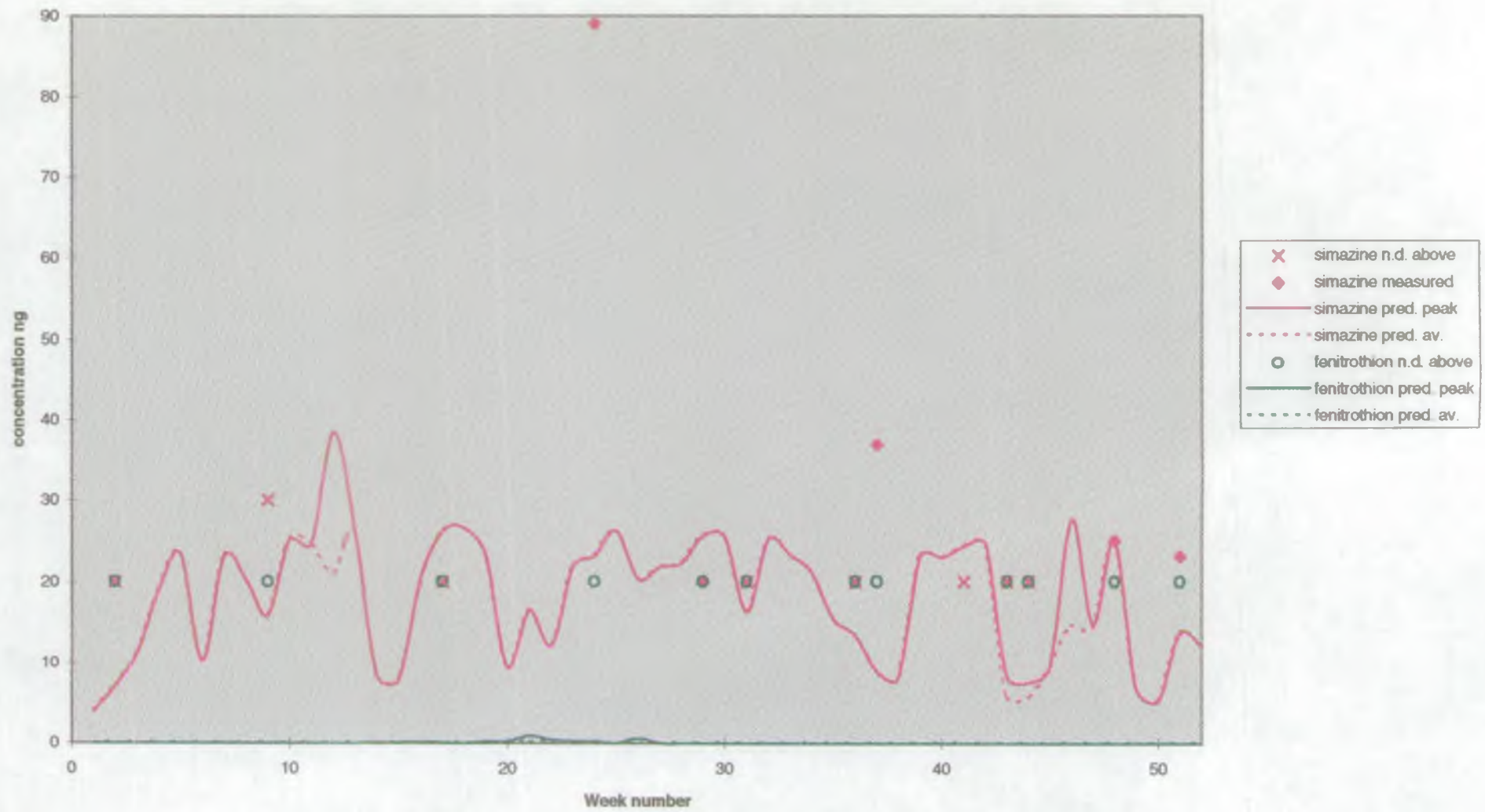
R. Otter 1994 gamma HCH & endosulfan concs.

Legend:
- **✕** gamma HCH n.d. above
- **◆** gamma HCH measured
- —— gamma HCH pred. peak
- ····· gamma HCH pred. av.
- **○** endosulfan n.d. above
- —— endosulfan pred. peak
- ····· endosulfan pred. av.

x-axis: week number
y-axis: concentration ng
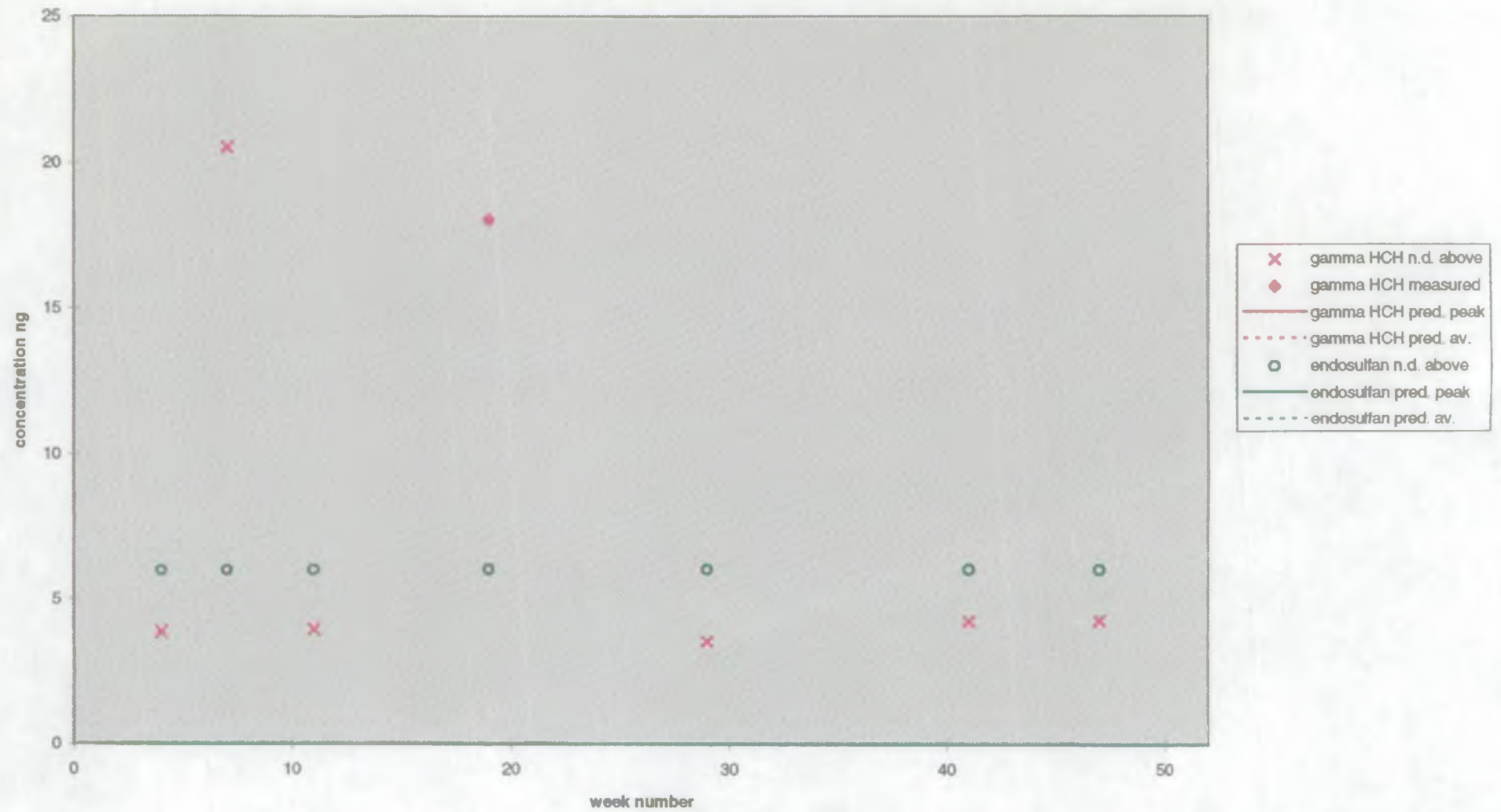
R. Hayle 1994 IPU & simazine concs.

Legend:
- ○ simazine n.d. above
- —— simazine pred. peak
- ······ simazine pred. av.
- ✕ IPU n.d. above
- —— IPU pred. peak
- ······ IPU pred. av.

y-axis: concentration ng

x-axis: week number
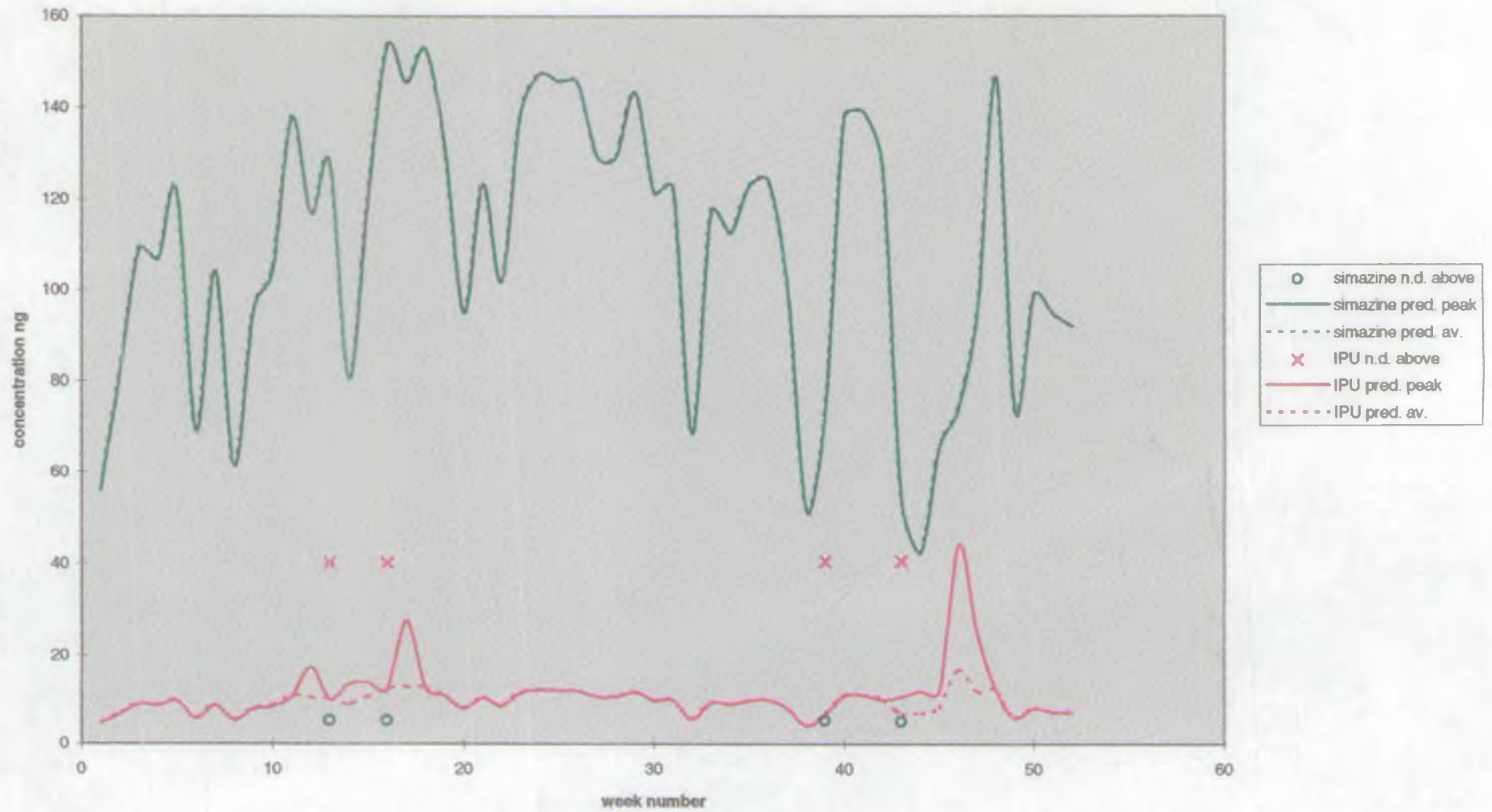
R. Hayle 1994 gamma HCH & chlorfenvinphos concs.

R. Severn 1994 IPU concs.