CSIRO
MARINE RESEARCH

Dissolved Oxygen Processing Notes

RV Southern Surveyor Voyage SS 02/98

11th March – 27th March 1998

Data processing completed by

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8 September to 9 September, 1999

Contents

1 Summary

These notes relate to the production of calibrated dissolved oxygen data for the *RV Southern Surveyor* voyage SS 02/98.

The dissolved oxygen sensor was calibrated using bottle data collected on the voyage and software written by Lindsay Pender ("procDO"). The bottle data had been processed prior to commencing calibration.

2 Voyage details

The following information is taken from the Data Centre's Marlin on-line data information:

Southern Surveyor cruise SS 02/98 had the objective of mapping the distribution of temperature, salinity, oxygen, nutrients and velocity in the vicinity of the Subantarctic Front, in the Southern Ocean south of Tasmania (approx. latitude 48 degrees-52 degrees S, 138 degrees-145 degrees E). Upper ocean currents are to be studied with ADCP and continuous measurements of sea surface salinity and temperature will be obtained from the salinograph for the whole voyage. Two magnetometer moorings were also to be recovered.

2.1 Chief scientist

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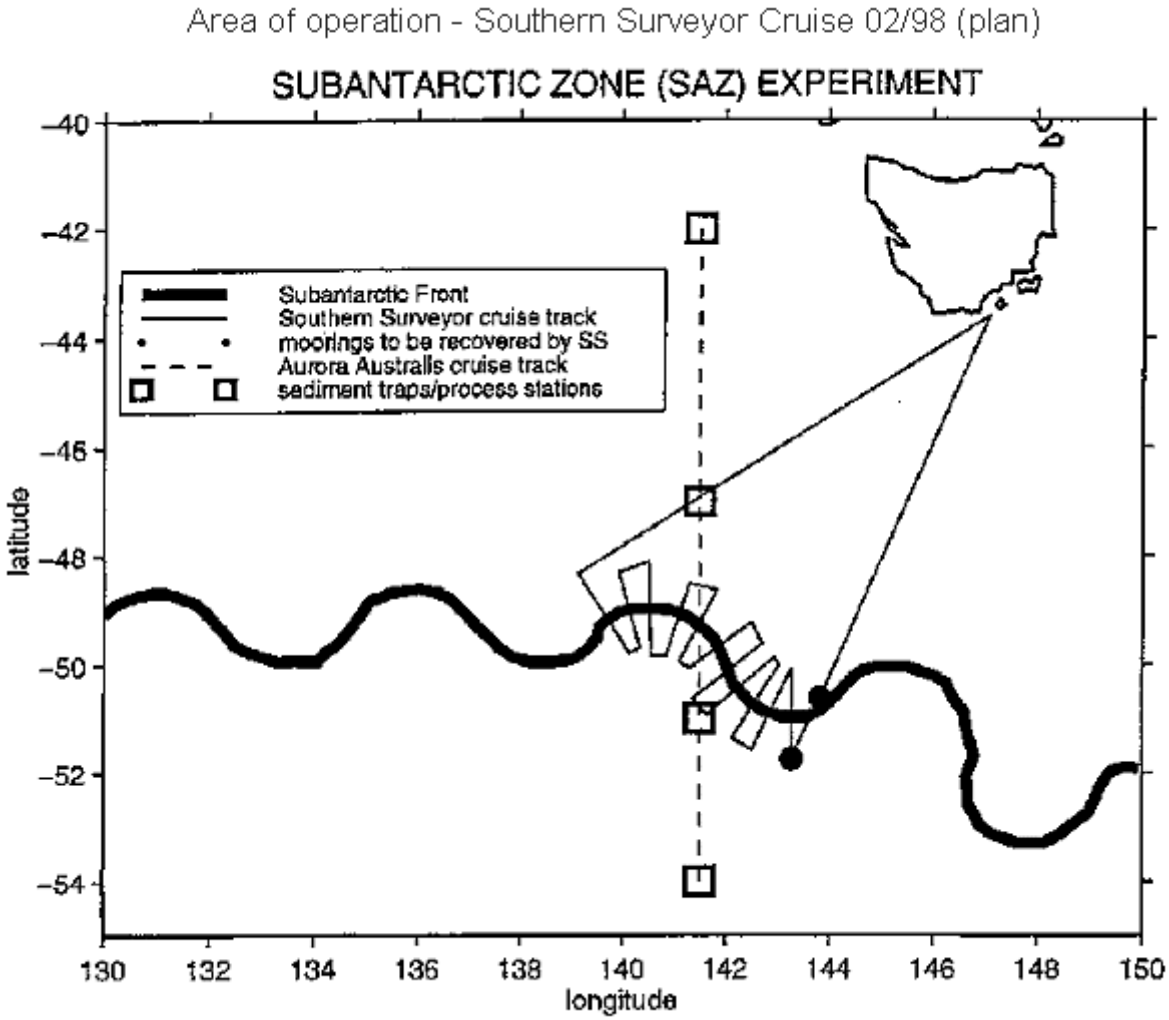
Figure 1 Voyage track



3 Processing notes

3.1 Introduction/background information

The dissolved oxygen sensor data was calibrated according to the on-line help associated with the processing software. The fitted model used was based on the model described by Atkinson, et al. (1996). The sensor type fitted to the CTD unit is an amperometric type, eg, Beckman model.

The dissolved oxygen sensor is attached to the CTD package which is lowered through the water column. Data is collected on the downcast, while bottle DO samples are collected on the upcast. Problems are encountered with matching of the bottle data with the downcast data due to: the flow rate sensitivity of the sensor (data collected on the downcast is at a high flow rate, while bottle data is collected while the CTD is stationary), movement of the ship during a cast means that the CTD may be passing through different water bodies, changes in the sensor used during the voyage.

To match the bottle data with the sensor data, it is assumed that the CTD downcast and upcast pass through the same body of water, which can result in some bottle data being

flagged as invalid, when in fact, the data is perfectly OK. During the regression stage of the processing, the model parameters can be either fixed or made free to be fitted. The regression is an iterative process based on the Levenberg-Marquardt method, and the casts can be grouped if necessary.

The CTD unit used on the voyage was #12. At the beginning of the voyage, a new automated DO titration system was installed for analysing bottle DO samples, but due to various technical problems, the system was not used. For the duration of the voyage a "hybrid" version of dissolved oxygen titration was used, with all the chemistry and other hardware of the new system, and a Vitex endpoint (as used in the manual titrations).

No dissolved oxygen data was available for casts 1 and 2.

4 Calibration and processing details

4.1 Bottle/sensor matching

Bottle data was matched with DO downcast data based on potential temperature from the downcast being matched with potential temperature on the upcast. The software automatically removes bottle data that fails a misalignment test. Bottles that are more than 1.5 times the standard deviation from the centroid are removed. This data is listed in Table 1.

Further to data that is automatically excluded, the processor is able to flag data as 'bad', or give individual bottles a weighting of between 0 and 1 so as to produce a better model of the sensor data. These edits are available from the file *S9802.oxy.bottleStatus*. Similarly, a listing of edited oxygen sensor current data is available from the file *S9802.oxy.ctdStatus*. Both files are large and are therefore not included in this report (contact Terry Byrne or Rebecca Cowley for these files).

Table 1 Invalid bottles removed from dissolved oxygen processing list.

The following bottles did not adequately match CTD casts.

Cast	Bottle	Error	Cast	Bottle	Error	Cast	Bottle	Error
3	5	0.015	28	12	-0.261	67	6	0.055
4	5	0.016	28	11	-0.258	68	10	-0.240
4	3	0.009	29	8	0.071	69	4	0.031
6	3	0.010	29	4	-0.005	71	12	0.208
7	12	-0.230	30	12	-0.285	71	11	0.205
7	11	-0.228	30	11	-0.280	71	1	-0.006
7	10	-0.113	30	10	-0.277	74	11	-0.285
7	9	0.313	30	9	0.097	74	5	0.011
8	12	-0.212	30	3	-0.021	75	12	-0.189
8	11	-0.212	31	10	-0.044	75	11	-0.200
8	10	-0.211	31	9	0.074	75	10	0.059
8	2	0.022	31	8	0.110	78	10	-0.080
9	11	-0.187	31	5	-0.009	79	10	0.089
12	10	-0.058	32	9	0.147	79	4	-0.009
12	9	0.128	32	2	0.010	80	12	-0.284
12	5	0.010	33	5	0.029	80	11	-0.272
12	3	0.012	37	9	-0.042	80	10	0.063
13	10	0.340	39	3	0.009	80	5	0.009

Cast	Bottle	Error	Cast	Bottle	Error	Cast	Bottle	Error
13	9	0.385	40	9	0.247	81	8	0.117
14	5	0.016	40	1	-0.005	82	10	-0.099
15	12	-0.269	41	2	-0.018	82	2	0.033
15	11	-0.268	44	10	-0.056	84	8	0.059
15	10	-0.069	45	10	0.057	84	7	0.060
15	7	0.061	45	4	0.017	84	5	0.022
16	5	-0.015	47	8	0.131	85	9	0.085
16	4	0.025	47	5	0.065	86	5	-0.044
16	3	-0.010	47	1	-0.007	87	10	-0.188
17	9	-0.086	48	5	0.018	87	4	0.009
17	8	-0.044	49	9	0.300	88	10	-0.101
17	5	-0.032	50	12	-0.192	88	9	0.308
18	9	-0.115	50	10	-0.187	88	8	0.214
18	8	-0.130	51	9	0.056	89	2	0.026
18	5	0.028	51	6	0.075	90	3	0.017
19	8	-0.141	52	10	-0.249	91	4	0.029
19	5	-0.007	52	1	-0.006	93	9	-0.043
19	4	0.012	53	9	0.073	93	1	0.011
19	3	0.035	53	5	0.014	94	6	0.299
19	2	-0.009	54	10	-0.041	94	4	-0.005
20	7	0.063	55	10	-0.169	95	11	-0.213
20	3	0.016	56	9	0.137	95	5	0.010
21	7	-0.080	56	8	-0.045	96	4	0.015
21	5	-0.015	56	5	0.036	97	1	0.009
22	4	0.019	56	3	0.009	99	6	0.067
23	12	-0.273	57	9	-0.040	99	5	0.045
23	11	-0.272	61	10	-0.243	100	7	-0.041
23	9	0.222	62	3	-0.010			
24	9	0.215	63	12	-0.225			
24	8	0.065	63	10	-0.057			
24	5	-0.010	63	9	0.293			
24	3	-0.055	64	12	-0.245			
26	12	-0.215	64	11	-0.241			
26	11	-0.216	65	12	-0.260			
26	10	-0.215	65	11	-0.260			
26	2	-0.006	65	2	-0.009			

4.2 Sensor model parameters

The oxygen sensor data was initially grouped into three so as to give a better regression fit. These groups were 3 to 14, 15 to 20 and 21 to 101. After flagging and weighting more bottle data points to get a better fit, the groups were extended to: 3 to 14, 15 to 20, 21 to 30, 31 to 41, 42 to 46, 47 to 65, 66 to 86 and 87 to 101 (a total of eight groups).

The final regression parameters were checked for physical reality, and tables 2 to 9 give the parameters for each station grouping.

Figure 2 Bottle data fit, post-processing.

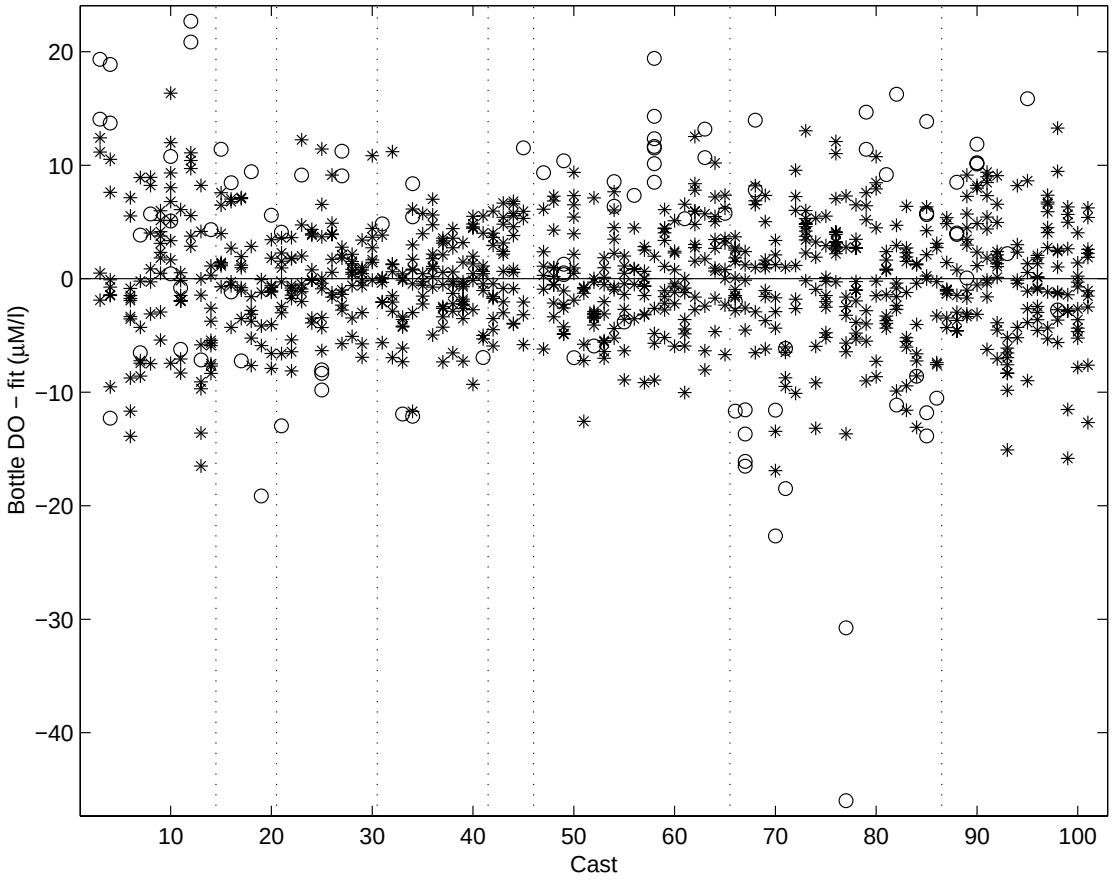


Table 2 Regression statistics for stations 3 to 14.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R'T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00037594 ± 0.000237	Yes
p_3	6.3188 ± 0	No
p_4	0 ± 0	No
p_5	−6.0886e−06 ± 8.988e−06	Yes
p_6	4829.2 ± 364	Yes
p_7	−21.09 ± 6.217	Yes

Cast range: 3 − 14
Number of available bottles fitted: 88
Number of bottles flagged bad: 17
Number of iterations: 3
Standard derviation of fit (weighted): 5.776
Standard derviation of fit (unweighted): 6.932
Date: 13−Sep−1999 11:15:31

Table 3 Regression statistics for stations 15 to 20.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R^{'}T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00038994 ± 0.0004079	Yes
p_3	10.15 ± 4.484	Yes
p_4	0 ± 0	No
p_5	−4.6063e−06 ± 9.901e−06	Yes
p_6	4781.4 ± 591.5	Yes
p_7	−32.884 ± 7.257	Yes

Cast range: 15 − 20

Number of available bottles fitted: 41

Number of bottles flagged bad: 7

Number of iterations: 3

Standard derviation of fit (weighted): 3.806

Standard derviation of fit (unweighted): 4.366

Date: 13−Sep−1999 14:24:43

Table 4 Regression statistics for stations 21 to 31.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R^{'}T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00032672 ± 0.0001758	Yes
p_3	4 ± 0	No
p_4	0 ± 0	No
p_5	2.7757e−06 ± 2.763e−06	Yes
p_6	4899.2 ± 307.8	Yes
p_7	−41.156 ± 5.21	Yes

Cast range: 21 − 30

Number of available bottles fitted: 84

Number of bottles flagged bad: 8

Number of iterations: 3

Standard derviation of fit (weighted): 3.365

Standard derviation of fit (unweighted): 4.009

Date: 13−Sep−1999 14:24:51

Table 5 Regression statistics for stations 32 to 41.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R'T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00030863 ± 0.0001966	Yes
p_3	4 ± 0	No
p_4	0 ± 0	No
p_5	$-1.5344e-05 \pm 1.342e-05$	Yes
p_6	4865 ± 364.1	Yes
p_7	-13.986 ± 6.183	Yes

Cast range: 31 − 41

Number of available bottles fitted: 100

Number of bottles flagged bad: 12

Number of iterations: 2

Standard derviation of fit (weighted): 3.226

Standard derviation of fit (unweighted): 3.841

Date: 13−Sep−1999 14:24:56

Table 6 Regression statistics for stations 42 to 45.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R'T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00031758 ± 0.0003104	Yes
p_3	4 ± 0	No
p_4	0 ± 0	No
p_5	$-1.0381e-05 \pm 1.587e-05$	Yes
p_6	4889.8 ± 559.2	Yes
p_7	-12.222 ± 9.648	Yes

Cast range: 42 − 45

Number of available bottles fitted: 36

Number of bottles flagged bad: 3

Number of iterations: 3

Standard derviation of fit (weighted): 3.8

Standard derviation of fit (unweighted): 4.376

Date: 13−Sep−1999 14:25:02

Table 7 Regression statistics for stations 47 to 65.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R'T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00032896 ± 0.0001434	Yes
p_3	7.0646 ± 2.435	Yes
p_4	0 ± 0	No
p_5	−1.0197e−06 ± 2.932e−06	Yes
p_6	4884.8 ± 248.9	Yes
p_7	−31.271 ± 3.417	Yes

Cast range: 47 − 65

Number of available bottles fitted: 158

Number of bottles flagged bad: 30

Number of iterations: 3

Standard derviation of fit (weighted): 4.013

Standard derviation of fit (unweighted): 4.535

Date: 13−Sep−1999 14:25:08

Table 8 Regression statistics for stations 66 to 86.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R'T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00033313 ± 0.0001492	Yes
p_3	11.697 ± 1.974	Yes
p_4	0 ± 0	No
p_5	−1.0669e−07 ± 2.755e−06	Yes
p_6	4878.6 ± 256.9	Yes
p_7	−32.844 ± 3.18	Yes

Cast range: 66 − 86

Number of available bottles fitted: 170

Number of bottles flagged bad: 35

Number of iterations: 3

Standard derviation of fit (weighted): 4.72

Standard derviation of fit (unweighted): 5.492

Date: 13−Sep−1999 14:25:15

Table 9 Regression statistics for stations 87 to 101.

Sensor Model

$$O_2 = ((p_1N+p_2)(I_O+p_3dI_O/dt)-p_4N-p_5)S_O(S,T,P)/(\exp(-p_6/RT)\exp(p_7P/R'T))$$

Parameter	Value	Fitted
p_1	0 ± 0	No
p_2	0.00033344 ± 0.000171	Yes
p_3	4.7183 ± 2.614	Yes
p_4	0 ± 0	No
p_5	−3.3367e−06 ± 5.268e−06	Yes
p_6	4861.6 ± 294.1	Yes
p_7	−29.902 ± 5.252	Yes

Cast range: 87 − 101

Number of available bottles fitted: 139

Number of bottles flagged bad: 15

Number of iterations: 3

Standard derviation of fit (weighted): 4.811

Standard derviation of fit (unweighted): 5.349

Date: 13−Sep−1999 14:25:22

4.2.1 Data Quality

The data calibration appears to be very good, with standard deviation of fit (weighted) ranging from 3.229 for stations 31 to 41 to 5.792 for stations 3 to 14.

5 References

Atkinson, M. J., Thomas, F. I. M. and Larson, N. (1996). *Effects of pressure on oxygen sensors.* Journal of Atmospheric and Oceanic Technology, 13:(6)1267,1274.

Processing completed by Rebecca Cowley on 13 September, 1999. Rebecca.Cowley@marine.csiro.au