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Validation of coastal oceanography at Laxemar-Simpevarp

Site descriptive modelling SDM-Site Laxemar

Anders Engqvist, Royal Institute of Technology (KTH)

Oleg Andrejev, Finnish Institute of Marine Research

December 2008

Svensk Kärnbränslehantering AB Swedish Nuclear Fuel and Waste Management Co Box 250, SE-101 24 Stockholm Tel +46 8 459 84 00



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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the authors and do not necessarily coincide with those of the client.

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Abstract

The Swedish Nuclear Fuel and Waste Management Company (SKB) is undertaking site characterization at two different locations, the Forsmark and the Laxemar-Simpevarp areas, with the objective of siting a geological repository for spent nuclear fuel. The characterization work is divided into an initial site investigation phase and a complete site investigation phase /SKB 2001/. In this context, the water exchange of the coastal zone is one link of the chain of possible nuclide transport mechanisms that must be assessed in the site description of potential repository areas /Lindborg et al. 2006/.

For the purpose of validating the pair of nested 3D-models and the coupled discrete basin (CDB-) model employed to simulate the water exchange in the near-shore coastal zone in the Laxemar-Simpevarp area, an encompassing measurement program entailing data from six stations (of which two are close) has been performed. The design of this program was to first assess to what degree the forcing of the fine resolution (FR-) model of the Laxemar-Simpevarp study area at its interfacial boundary to the coarse resolution (CR-) model of the entire Baltic was reproduced. In addition to this, it is of particular interest how the time-varying density-determining properties, salinity and temperature, at the borders are propagated into the FR-domain and further influence the water exchange with the interior, more secluded, basins. An important part of the validation process has been to carefully evaluate which measurement data that can be considered reliable. The result was that some periods of foremost near-surface salinity data had to be discarded due to growth of algae on the conductivity sensors. Interference with ship traffic and lack of absolute calibration of the salinity meters necessitated dismissal of measurement data too. In this study so-called Mesan data have been consistently used for the meteorological forcing of the 3D-models.

Relative the assessed data that can be accepted as adequate, the outcome of the validation can be summarized in three points: (*i*) The Baltic CR-model reproduces the measured salinity and the temperature profiles of the three peripheral stations acceptably well, while the correlation levels of the velocities are on an acceptable level for only one component, the other being close to zero; (*ii*) For the interior station Si24, the FR-model reproduces the salinity and the temperature profiles with a yet improved level of correlation compared with the CR-model; (*iii*) The bottom current velocity measured at Djupesund corresponds to an internal strait within the CDB-model and yields a correlation level of nearly 50% for salinity and about 95% for temperature.

The conclusion is that the present validation of *velocity* components of the peripheral stations between the CR- and FR-domains has mainly confirmed what was found in the corresponding validation study of the Forsmark area /Engqvist and Andrejev 2008/, namely that this represents a challenge that demands considerably more measuring effort than has been possible to muster presently in order to average out sub-grid eddies that the model cannot resolve. This applies even though the levels of the correlation analysis are considerably higher than was found for the parallel study of the waters off the Forsmark coast. This together with supporting current velocity transects in the vicinity of the measurement stations can be explained by a more horizontally homogeneous flow field. For the inner station (Si24) that was computed by the FR-model, the correlation levels are considerably improved. Also for the station (Si25) pertaining to the CDB-model good correlation levels are reproduced. All temperature profiles are also acceptably well captured by the models, but this is judged to be more an effect of the seasonal variation than an expression of the virtue of the actual models. As for the Forsmark validation program, the salinity dynamics of the interior FR-domain is the strong point of the model, but in the present study high levels of salinity correlations also extend to the peripheral measurement stations computed with the CR-model. Taken together this means that the overall earlier modeled water exchange of the Laxemar-Simpevarp caostal area can continue to be invested with due confidence.

Sammanfattning

Svensk Kärnbränslehantering AB genomför platsundersökningar vid två olika platser: Forsmarks- och Laxemar-Simpevarpsområdet. Syftet är att lokalisera en långsiktig förvaringsplats för utbränt kärnbränsle. Karaktäriseringsarbetet är uppdelat i två faser varav den första är en initial platsundersökning och den andra en komplett sådan /SKB 2001/. I detta sammanhang utgör vattenutbytet genom kustzonen en länk i en lång transportkedja av möjligt utläckande radionuklider /Lindborg m fl 2006/.

Ett omfattande mätprogram har genomförts i syfte att validera det par av två sammankopplade 3D-modeller som har använts för att simulera vattenutbytet i den strandnära kustzonen i Forsmarksområdet. Modellansatsen består av en grövre upplöst (GU-) modell över hela Östersjön och en finare upplöst (FU-) modell samt en kopplad diskret bassäng (KDB-) modell över det studerade kustområdet i Forsmark. Utformningen av detta program syftade i första hand till att utröna i vilken omfattning drivningen över gränssnittet mellan dessa två modeller bestämmer vattenutbytet i det inre högupplösta området. Utöver denna granskning, omfattande sex mätstationer, har det varit av speciellt intresse att se hur densitetsbestämmande egenskaperna salinitet (S) och temperatur (T) vid dessa modellränder propagerar in till de inre delarna av FU-domänen. En viktig del av valideringsprocessen har varit att noggrannt utvärdera vilka mätdata som kan betraktas som tillförlitliga. Resultatet blev att några företrädesvis ytnära salinitetsdata måste förkastas på grund av algpåväxt som inverkar menligt på konduktivitetssensorerna. Brister avseende absolutkalibrering av salinitetsinstrumenten har också medfört att vissa sammanhörande data måst utelämnas från den fortsatta statistiska analysen av uppenbara skäl. För den meteorologiska drivningen av 3D-modellerna har Mesandata använts genomgående.

I förhållande till de insamlade data som kan accepteras såsom rättvisande, kan resultatet av denna validering summeras i tre punkter: (*i*) GU-modellen över Östersjön simulerar de uppmätta salinitets- och temperaturprofilerna för de perifera mätstationerna på ett acceptabelt väl sätt. Motsvarande korrelationer för strömhastigheterna är tillfredsställande endast för en av de två vinkelräta komponenterna, medan den andra är nära noll. (*ii*) För den inre mätstationen Si24 vars värden beräknats med FU-modellen uppkommer korrelationsnivåer för salinitet och temperatur som överträffar de som erhållits med GU-modellen. (*iii*) Bottenströmhastigheten som uppmätts i Djupesund som motsvaras av ett internt sund inom KDB-modellen ger en korrelationsnivå nära 50 % för salinitet och omkring 95 % för temperatur.

Sammanfattningsvis har valideringen av *hastighets*komponenterna i stort bekräftat vad som har visats i många tidigare studier, nämligen att detta utgör en krävande utmaning som fordrar väsentligt större mätansträngning än vad som varit möjligt att mobilisera i denna studie för att kunna medelvärdesbilda över tids- och rumsskalor som modellerna inte upplöser. Detta gäller även om korrelationsnivåerna är avsevärt högre än vad som befanns för den parallella studien rörande Forsmarks kustvatten /Engqvist and Andrejev 2008/, vilket tillsammans med stöd av utförda strömhastighetstransekter kring de perifera mätstationerna, kan förklaras med ett mer sammanhållet homogent strömningsfält i horisontell led. Även om temperaturvariationerna har modellerats acceptabelt väl, hör detta också samman med den uttalade säsongsdynamiken. Salinitetsdynamiken utgör dessa modellers starka sida. Dess variationer reproduceras övertygande väl av denna modellansats inte enbart för den inre stationen (Si24) beräknad med HU-modellen, utan också för de som beräknats med GU-modellen. Detta gäller även för den station (Si25) som modellerats med KDB-modellen. Sammantaget betyder det att tidigare modellerat övergripande vattenutbyte för Laxemar-Simpevarpsområdet med tillförsikt även fortsättningsvis kan betraktas som trovärdigt.

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1 Introduction

1.1 The cascaded 3D-model approach

The Baltic model (AS3D) employed in this study /Andreiev and Sokolov 1989, 1990/ has been developed for the main purpose of providing insight into the circulation of the central Baltic. Its present horizontal resolution is set to $2' \times 2'$ (nautical miles) based on the Warnemünde hypsographic data, see Figure 1-1. This is conveniently referred to as the coarse-resolution (CR) model. In spherical coordinates the model spans the area defined by the southwest corner (53° 48' N, 9° 27' E) and the northeast (65° 52' N, 30° 27' E). The horizontal diffusivity is nominally set to 30 $[m^2/s]$, consistent with assuming the grid cells to be well mixed. This model is presently involved in several ongoing Baltic hydrographic studies /e.g. Andrejev et al. 2004ab/. A thorough testing of this model in comparison to measured data /Engqvist and Andrejev 2003/ revealed that along an interface to a model area comprising the Stockholm archipelago, the measured salinity and temperature profiles were acceptably well reproduced, with the main difference being an offset in salinity approximately evenly distributed over the depth range. This evaluation thus increased confidence in the realism of the AS3D model. The heat exchange with the atmosphere is mainly determined by the air temperature: likewise the ice formation and melting processes are formulated in a simple but straightforward manner. This would be a liability if the main concern were to correctly predict the ice situation /e.g. Omstedt 1999/. The ice dynamics is not a concern for the part of the Baltic coast that is situated offshore of the Laxemar-Simpevarp area, however. For projection into a distant future, climate scenarios could more likely supply a forecast of shifting air temperatures, while other factors determining the heat exchange (insolation, relative humidity and nebulosity) would probably be more inaccessible

The grid of the local fine-resolution (FR) 3D-model has been computed from a Digital Elevation Model (DEM) based on national digitized charts, complemented with shoreline information from economical maps. The grid has been specified in spherical coordinates WGS84 (sweref 99 long lat ellh) with the constraint that to be considered as a wet grid cell at least 50% of the covered area must consist of water. The numerical scheme is identical to the Baltic (CR) model but the horizontal diffusivity is nominally set to 20 $[m^{-2}s^{-1}]$ compared to 30 $[m^{-2}s^{-1}]$ for the Baltic model. The Laxemar-Simpevarp coastal area was resolved horizontally into grid cells with a side length of 0.1×0.1 nautical mile (Figure 1-2) defined by the SW corner with spherical coordinates (57° 20' N; 16° 31' E) and the NE corner (57° 32' N; 17° 03' E). The final choice of the actual model area includes a small section of the major island Öland in the SE corner. The inner more secluded embayments, e.g. those that surround the Aspö island, do not become sufficiently resolved with this resolution and their water exchange with the Baltic coast must therefore be computed using another model approach in the form of a coupled discrete basin model that will be referred to as the CDB-model. In fact, when using the objective gridding criterion that at least 50% of area must consist of water meant that these interior waters were disconnected in the FR-grid at a few locations. In order to attach these to the main computational domain, manual corrections were performed.

The CDB-model has been developed in stages since it was first applied to the basins adjacent to the Äspö island /Engqvist 1997/. Its present enhanced features have been described in /Engqvist and Stenström 2004/ and it has been successfully validated in the Himmerfjärden area about 40 km south of Stockholm /Engqvist and Stenström 2008/. This model will be presented in more detail in section 3.6 below that deals with the measurement validation of station Si25.

The overall objective has been to evaluate these three nested numerical models with differing resolution (CR, FR and CDB) regarded as an operational entity and to investigate their combined capacity to simulate the measured oceanographic data.



Figure 1-1. Baltic model bathymetry resolved into a grid with 2×2 nautical mile side length The fineresolution model of the Laxemar-Simpevarp area and its approximate location relative the Baltic model is indicated with a red rectangle. The open boundary of Baltic model falls where Kattegat borders to the Skagerrak.



Figure 1-2. Local fine-resolved model domain with red dots indicating the measurement stations where the oceanographic instruments were deployed during the validation year cycle starting in spring 2004. The labels denote the reference naming of these stations used in the text. The axes are graded in grid cell number with a horizontal resolution of 0.1 nautical mile i.e. 185.2 m.

1.2 Design of the field program

The general design idea of the field program was primarily to assess the oceanographic state parameters at some locations distributed as evenly as possible on the boundaries of the local model (FR-) grid which coincide with the interfaces to the nested (CR-) grid of the Baltic model. These stations are listed in Table 1-1 (their positions are shown in Figure 1-2) and are meant to represent the forcing of the large-scale events onto the fine-resolved local model domain. The oceanographic measurements consist of both vector entities, i.e. current velocities, and the scalar properties temperature and salinity.

Temperature is measured directly by use of thermistors but salinity is indirectly inferred from measured conductivity. All salinities in the following are presented dimensionless in the psu-scale. These two scalar properties determine (together with pressure) the density of the sea water. Assessment of these entities at the periphery together with the atmospheric heat exchange and freshwater discharge makes it possible to model their propagation into the center of the domain where an evaluation relative other measurement sites can be performed. The measurement procedures of oceanographical parameters have been specified by /Johansson and Morosini 2002/.

Based on experience from other similar validation endeavors, it was anticipated that for the scalar data, it should be straightforward to make a direct and fair evaluation, while vector comparisons would be considerably more difficult. In negotiations with the contracted executioner of the field program, Swedish Meteorological and Hydrological Institute (SMHI), bottom-placed ADCP-instruments were recommended over RCM-instruments that also normally can be equipped to measure salinity and temperature. The argument was partly that bottom-placed instruments are less vulnerable to interfering with other maritime activities and partly that they are less expensive to deploy and operate.

In order to secure data, the one-year measurement period was subdivided into four sections with approximately equal duration but open to allowances due to poor weather conditions and other incidents that are difficult to apprehend. This plan was specified in detail in the Activity plan AP PS 400-04-10 with Karin Aquilonius as the contemporary SKB representative.

Table 1-1. Overview of the naming and locations of the measurement stations. The RT90 coordinates differ from corresponding positions stated in /Lindow 2005/. For the measured entities C denotes conductivity, T temperature and D direction. U and V denote current speed components.

		Station ID			Position			Depth	
Location name				Northing	Easting	lat	long	desired	realized
	Measured entity	SKB	SMHI	(RT90 2.5 g	gon V (0:-1	(WGS 84 S	Sweref 99)	[m]	[m]
				RT90 data	from P-05-				
North boundary E	4xC/T	PSM6927	Si21a	6377920	1566900	57° 32.0'N	16° 55.5'E	~40	66
North boundary W	U,V	PSM6928	Si21b	6379016	1565837	57° 32.0'N	16° 54.5'E	~40	42
East boundary	C/T/U/D	PSM6929	Si22	6368104	157496	57° 26.0'N	17º 03.0'E	~50	50
South boundary	U,V	PSM6930	Si23	6356926	1559731	57° 20.0'N	16° 48.0'E	24	26
Inner station	3xCT	PSM6931	Si24	6368855	1558314	57° 26.5'N	16° 46.8'E	20	28
Inner station (non-ice	cover time) 11xT	PSM6931	Si24T	6368855	1558314	57° 26.5'N	16° 46.8'E	~20	28
Djupesund	C/T/U/D	PSM6932	Si25	6369500	1552493	57° 27.0'N	16° 41.0'E	~6	4.2

1.3 Overview of the measurement program

The measurement program was originally planned to start on January 1, 2004, but due to various reasons, e.g. the ice situation on the parallel program of Forsmark, this was delayed until mid-April the same year. In Table 1-2 the field program is specified in detail regarding the measured parameters and their deployment with regard to depth. This table also gives a first rough presentation of the data yield and also lists the names of the resulting 83 data files.

It seems safe to state that the actual handling and deployment of the instruments has been conducted professionally and with due care. The handling and communication of data has, on the other hand, left more to be desired. Initially there was a complete abandonment of the specified protocol, and even in the same file (e.g. time denoting), the data format could be changed several times. No inspection of the presumed validity of data was performed by SMHI, but the chore of quality inspection was passed over to be performed by SKB. It is also fair to state that by the end of the validation year, the accumulated criticism also led to a noticeable improvement in SMHI's performance in this regard.

The report on the assessment of oceanographic data conducted by SMHI /Lindow 2005/ admits most of the shortcomings, but not all. In Table 1-3 some of the additional sources of consternation have been commented upon.

1.4 Validation strategy

The overall validation plan is straightforward and consists of first inspecting the measurement data to dismiss the sections that for various reasons cannot be trusted. Then follows an investigation of the spectral appearance of the remaining data in order to determine an appropriate sampling frequency for the ensuing comparison with matching simulated data. Finally the actual comparisons are performed, which in most cases result in cross-correlation analysis. The five measurement locations, Si21 through Si25, are treated in order.

Table 1-2. Overview of the naming of the data files and what measured entity they denote. Gray fields indicate data problems, see Figure 2-1 for an explanation.

					File			
period			Depth		number	SMHI file name	Systematic name	SICADA_06_104_2
140	Si21a	PGM0027	2 m CT	O T.C	1	00E37.021_2m.sta	0x21_1eM_111_TC_02m.cm	
191		PSL8927	10 m CT	DIC	2	SBE37 5421_10m xis	\$121_1#4_N1_TC_10m_csv	
181		PSM8327	17 m CT	D T.C		missing	in the second	
141	1.1	PS149927	30 m CT	D TC	3	\$8E37 5(21_30m sta	Si21_1el4_N1_30en_TC cev	
and		P\$100027	2 m (CT	D T.C	4	SBE37 SQ1 2m.sla	\$421 2x44 N1 TC 02m cev	
200		PS449327	10 m CT	D T.C	5	SBE37 Si21_10m xis	Si21_2e4 N1_TC_10m cm	
2nd		PS1/6927	17 m CT	D T,C	6	SBE37 Si21_17m xla	Si21_2el4_N1_TC_17m.cev	
2nd		PS1/8927	30 m CT	D TC	7	SBE37 SQ1_30m x14	\$121_2x44_N1_TC_30m_cev	
310		PSU8927	2 m CT	D TC&D	8	\$21 Jm xlp	Sign Jaté N1 10 03m cev	
340		PSM8927	to en CT	D T.C	9	3/21_10m.xlp	3/21 Jul4 N1 TC 10m cav	
340		PSM927	IT m CT	D T.C	12	S-21_17m.xte	Si21 Jell N1 1C 1/m cev	
3id		PG140327	30 m CT	D T.C	15	Gigt 36m xta	0i21 Juli N1 TC 30m cav	
49		PSL8927	5 m CT	D TC&D	12	5-21-4 SBE37-130 Sm x8	SQ1 Anti N1 1C Olim cov	
40	-	PGM6927	10 m CT	DIC	13	8/21-4 SBE37-129 13m x	Si21 4el4 N1 TC 10m csv	
427		P5149927	IT m CT	DIC	14	5/21-4 58E37-124 17 Ser	Si21 4H4 N1 TC 17m cm	
40		PELM027	30 m CT	DIC	15	621-4 58E37-126 30m x	Si21 Juli N1 TC 30m cov	100000
	\$4210	P516928	3 2 39 mAD	CP 15xU	15	\$21 101 V1 Hot K9	SIZ1 168 NT U M CRV	OC105current east aduated cev
140		PELADORE	3 2 30 mAD	CP 15xV	17	0.01 101 V2 kov.xls	Di21 1pH N1 V cav	OC140 current north acuados cau
541		PSLA9328	3.2.39 mAD	CP 19v1V	15	SQ1 101 V3 kov vis	Si21 1ett N1 W cm	
141		PEMegge	1	3 PT		mission	1.000	
		PSLMICE	\$ 2.39 mAD	CP 15xU	15	5/21-201 v1 xis	5(21 2ml4 N1 U cm	OC145-current wast aquadop cav
2nd		PELNOCU	0.2.30 mAD	CP 15xV	23	6/21-201 v2 xts	Si21 2nd N1 V cav	OC14i/current north aquados cau
200		PSIM928	0.2 33 mAD	CP 19vW	21	S(21-201 v3 x8x	Si21 2el4 N1 W cm	OC145icurrent up aparation cav
200		PSIA928	1239 mAL	CP 15vU	22	8/21-301 v1 sta	Si21 2ett 1/2 U etv	OC145/current aast aquadop cov
200		POLMACO	0 2 30 mAD	CP 15xV	22	3/21-301 v2 xla	321 2x4 112 V cm	OC140 current moth assurator cause
200		PSLAVICE	0.2.39 mAD	CP 19vW	23	5/21-301 v3 stg	1921 2ntl 102 W.cm	OC188 current un asuadon env
200		PSIMISON	and shall be seen in the second	PT	24	321 201 see als	Si21 2n4 N1 PE cm	
200		PS14903	0.0000	PT	25	SQ1 301 see via	Si21 2Ht N2 PT Ht	A STATE OF A
-		PCLASSOF	2242 m 42	CP 20xU	28	0.01-401 v1 v1a	Di21 Jold N1 U cav	OC140 current east acuados car
let		PS14926	3243 0 40	CP 20xV	27	5(21,431 v7 via	Si21 Juli N1 V cm	OC145 current parts as accer can
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and		P-34834/3	-	BUDCIS		Distant	And a la fit sector in	1
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-0	-	P-25/0323	47.71 5%	4 001	12	312-4 A#330.30-4319.419	022 4#4 E1 001- 49m C	Pr
141	5423	P\$190000	0224 m A0	QP 1280	25	5/20_101_V1 xis	5423 10% 51 U cov	OC140/CUNINE_BASE_BWBC COV
197		PS449930	0 2 24 m AD	CP 128V	37	5/23_101_V2 x88	5423_1044_51_V C8V	OC140 CANNUE NOTING CAN
181		PS1/6930	0224 m AD	CP 12KW	35	SQ3_161_V3 x88	5k23 1eH 51 W.cev	OC140/currents_uplesv
16		PSM0320		PT		gnistim		
and		PS149930	2224 m A0	CP 12x0	39	\$423-201_v1 xig	\$23_2#t1_\$1_U.cev	OC100/current_east_awac.cov
210		PGM6900	2.2.24 m AD	CP 12KV	40	3/23/201_V2 xhs	3/23_2//4_31_V cm	OC140 current_norting.cav
200		PS18930	2226 m AD	CP 12XW	41	\$43-201_v3.stu	5i23_2i48_51_W.cev	OC100/curseres_up.cev
Suc	-	P\$440300	2224 m A0	Ch (540	42	9/22-301_v1 xts	D23_2v4_02_0 cm	OC140/current_east_awac.cav
200	-	PS149930	2.2.24 m AD	CP 12xV	43	S/23-301_v2 ste	\$123_2044_\$2_V.cev	OC140 curvers_nothing cav
2nd		P6446930	2224 m AD	CP 12VW	44	8/23-301_v3 xla	8k23_2w4_82_W eev	OC140/currents_up.cav
and		PSIMIOC	7.7.24 m AD	CP 12x0	45	8/23-401_v1 x18	\$423_7#4_53_0 cm	OC140/current_east_awac car
and		PSUMBOO	2224 m AD	CP 12xV	45	\$23-431_v2 xlp	\$423_2#M_\$3_V.cev	OC140/current_northing.cov
210		PSM9900	2.2.24 m AD	CP 12/W	47	3/22-401_v3 xls	3/22 2/44 33 W cav	00140cuments_up.cm
210		PSM6930	1000 L	P.T.	45	5/23-201_een.xte	5123_2010_51_PT.cov	
200	-	P\$M0300		PT	40	0.22-301_sen.xts	0/22_2vH_02_PT can	
2nc	-	PSLM930		PTAC	50	5/23-431_san x/s	523 2m4 53 PT cov	
310	_	PEMeggo	2.2.28 m AD	CP 14x0	- 51	6/23/302_v1 xla	6i20_3eH4_61_U eav	OC140/current_east_awac.cov
345		P514930	2 2 28 m AD	CP 14XV	52	5/23-302_v2 sta	5i23_3et4_51_V etv	OC100curers_hotting.cev
340		PSIA0000	2228 m A0	CP 14xW	53	5-22-302 v3 xla	Sk23 Johl S1 Wicov	OC140 currents up cav
30	-	PSLARA		PT&C	54	8/23-301 set k/s	8(2) 304 S1 PT (pr	
48		P516930	2226 m AD	CP 12x0	55	823-4 AMAC VI MB	5i23_4#4_81_U.eav	OC140/current_east_awac.cov
40		P\$\$40930	2.2.26 m AD	QP 12xV	- 56	342-4_AWAG_v2.xla	323_4eH_51_V cai	OC140 current_northing cav
491		PSLA9900	12 2 26 m AD	CP 13xW	47	Sight AWAC visite	5423 Apt1 \$1 W.cp/	Octoccutents up cov
40	-	PS146930	28 m	PISC	58	SI23-4 AVVAC service	13(2) 4#4 S1 PT etv	
191	5024	P\$149971	2 m CT	0 1,0	69	\$86137_\$124_2m.xie	Sigi 1ett It TC 02m cev	· · · · · · · · · · · · · · · · · · ·
191		PSM6931	10 m CT	D T,C	- 60	88E37_824_10m.xlb	Si24_1el4_11_TC_10m car	
197		PS109931	17 m CT	D T,C	61	SG4_17m.xH	5124_1644_01_TC_17m cm	1
210		P\$140021	2 m CT	D T,C	62	5/24 2m.sta	804 204 11 02m TC cm	
2nd		PSL0971	tom CT	D T,C	43	S.24 10m sls	\$24 2#4 It 10m TC cm	
2nd		P6446031	I'n ci	D T.C	55	8/24 17 5m via	5/24 2#4 11 17# TC cov	
310		P514931	Zm CT	DIC	- 66	5/24 2m sls	5424 3el4 11 TC 02m cm	
340		PS14901	10 m CT	0 1,0	67	SQL 10m xlo	Size Jett 11_TC_10m.cev	
34	-	PS1/0901	1 n C	D T.C	- 53	3/24 17 Ser. Kit	324 Juli 11 TC 17m cm	
481		PS16931	5m CT	0 1,0	53	504-1 SBE37-127 541 x8	Size 466 IT TO Dom day	
40		PS140001	10 m CT	0 1,0	70	5-24-4_20C37-128_5m.xl	Digit 4pH II TO 10m cev	
49		PSL0971	IT et CT	0 T.C	71	SQL4 SBE37-125 17 Sm	S24 Juli II TC 17m cm	
141	SIZAT	PGM0001	1221 m TK	1taT	72	0.24_T_1.xla	QiQi 1pli 11_TK cav	-2
2nd		PSL49971	1221 m TK	1187	73	73035 St24ju8-sept 2004 x	SIG4 2044 II TK cov	
310		PEM6931	1221 m TK	11sT	74	AsT3040 8/24T Mb	8i24_3el4_11_TK.esr	
49		PS14931						
191	5425	PSM6932	4 m R0	W+UDCTS	75	s4_dupesurd.xts	Si25_1el4_D1_UDCT cev	
200			4 m RC	M+UDCT	76	5/25_640928 Mit	\$125_2#4_D1_UDCT cev	1
Jic		P\$140002	4 m R0	M+UDCT	77	6Q5 3.xts	Si25 Jolf D1 UDCT cm	
49		PSLM932	4 m 80	W+UDCT	78	\$254 54 xis	S25 4#4 D1 UDCT cm	
	Transe	cts					-	
04		-	10	CP	72	Singlife 20		
100		_	1	CP.	83	Same 7 2 m (19)		
201	-	_	1	CP.	14	Barr 100-000		
410	<u> </u>	_			41	1000.000	Demissal dia in continue	adhora
340	-	_	-	28		alar. 842, 555	Paragages one to nearly of c	
40			AQ	QP .	92	stabooel 000		
			AL AL	U.F	4.5	B1400014.000		

Table 1-3. Overview of the temporal aspect of the data and ensuing remarks and responses of the executioner of the field program. Gray fields indicate data problems that are explained in the three last columns.

Station	10					-			-	File	-	SAMP	SILH reporting
SALES.	BRANKS P	period	Depth	675	7.0	Mart 1	1	1000	10	number	Keihalla	response	15-40-191
36/1	P-38.86927	Tel	11.00	CTD	TC	23343331		20040708	0	9	re-ting conductivity unit	Consciso .	11
	PSMM227	1st	17 m	CTD	TC	1 million	and a		and the	-	Masing	Sector Action	Missing
	PSM4827	1 pt	30 m	CTD	1.0	20043335	. 15	20010706	. 1	3	Environments devidently values	Instrument replace	Net noted
-	PSMM927	2nd	2 m	CTD	T.C	23343737	. 11	20010929	10	4			
	PSMM927	2nd	13 m	CTD	T,C	20040707	11	20040929	10	6			
_	P:SM6927	2nd	17 m	CTD	T.C	23343707	11	20040929	10	6			
_	PSA46927	244	33 m	CID	10	22340707	1.11	20040122	- 2	1	Erroelatic contectivity values	Acknowlegded	
	P'5826827	210	278	CID	TCAD	220941001	11	20041107			DHee to 25m 2004-111-07 01-021/8	nit by ship acknow	
	P-9446927	20	17.00	CTD.	40	20041001		20061107		13	Locardan capta anal 2004, 11 (0)	Color alian accept	
	P-0446527	24	32 m	CTD	TC	20041001	11	20050111	10	11	Cross des regis e de reservoires	Construction accept	
-	PSM6327	419.	5 m	CTD	TCAD	20060114	15	20050406		12	Pressure unit in ted		Spikes in C: CTD of N
	P\$M6827	418	10 m	CTD	T.C	23060114	16	20060406		13			
	PSM#927	418	17 m	CTD	T,C	20060114	15	20050404	8	14			
	PSMM927	418	30 m	CLD	T.C	20050114	15	20050406	0	15			
\$121	P5636923	fat	37.39 #	ADCP	that!	20040401	. 9	20040706	1	15			
	P0836323	Tet	32.30 #	1 ADCP	Mat V	20040401	- 2	20040700	7	17	-	Statute and	
	P\$14929	1pt	3239 8	ADCP	19876	20040401	- 7	20040106	- 1	. 14	File initially confused	Pile replaced	Alleria
	010300020	100	1	40.00	There are a second at second at a second a	******		20010811	13	12			Viceng
	P-56/65/23	2nd	3 2 39 .	ADCE	1000	20040707		20040011	- 12	25	-		
	P-5636323	2nd	32.39 -	ADCP	that's	20040707	44	20040811	13	21			
	P-3646923	2nd	3 2 39 #	ADCP	1910	20040019	- 6	20040912	19	22			
	PSM6929	2nd	82.39 #	ADCP	15xV	20040819	6	20040912	19	22			
	PSM6929	2nd	32.39 #	ADCP	1900	22043819	6	20040912	19	23			
	PSM6828	2nd	8		P.T	23343737	12	20040811	14	24			
	PSM4928	2nd			PT	20083819	6	20010913	20	-25	triaking data, no units atabet	Instantant Inspected	
-	P3446921	3.0	22430	ADCP	20.0	29041002	14	20050112	10	25		1.	
-	PSMM321	34	2241 n	ADCP	20xV	29041002	- 14	20050112	10	27			
-	P'SN#925	24	0.243 m	ADCP	41271	22341232	14	20039112	10	25			
	P3846323	310	2.2.37	4000	1P.1	20041002	14	20050111	11	11	New rest in the second second second		
	P-SAMA71	4.8	3 2 37 0	ADCP	State V	23050114	1	20050413	12	31	the restored by space of		
	P3646928	416	3 2 37 1	ADCP	SBaW .	20050114	14	20050413	14	32			
	PSM6929	418	1 Contraction of the local division of the l		PT	20050114	14	20050413	1 12	33	Pressure and in Inf		
\$122	P\$116323	1pt.		RCM-	UDCTS	2	-	17					water leak
1	P\$14929	2nd			UDCTS								clock anor
	PSM4929	34	58 m	RCM-	U.D.T.C.S	20041020		20050127	. 9	34	Balanet bet for a panel		instrument racie-ed
	P.SAM829	418	43 m	RCM	UDT	20060304	14	20050309	21	34	Wank only 1. days - No kalony		pain they have to shall
\$173	P.5626333	161	0724 m	ADCP	1340	73043331	17	20040106	11	38	-		
-	POM/6333	192	0.2.24 m	ADUP	14XV	23343331	14	20040106	11		-	-	
-	P-3424333	100	N 6 64 H	AUCH	P T	2000 1001	-14	20040104	11	- 10			lind calibration
	P.SAJ4833	2nd	2224 0	ADCP	12xU	20043737	14	20010811	10	19	-		per calleraren
	P3M6930	2ml	2224 1	ADCP	12xV	23040707	16	20040811	10	43			
	PSM0930	2nd	2224 m	ADCP	12xW	20040707	16	20040011	10	41			
	PSM6933	2nd	2.2.24 m	ADCP	12x0	20040811	13	20040819	6	42			
	P5136930	2nd	2226 m	ADCP	12xV	20090811	13	20040819	6	43		1	
	P5636933	2nd	2224 0	ADCP	52xW	20040811	13	2004.0819	6	44			
-	P3030333	Zed	2 2 24 11	ADCP	17x0	72040019	- 2	20041001	13	45			
	P-36J63JJ	200	2234	ADCE	14XV	20040812		20041001	10	49			
	P-5836933	2nd		(Pray ar	PT	20343737	10.94	20010511	11	13	Value 1/Caster 10	Advestated	tases out of other
	P3446333	2nd		-	PT	20040011	13	20040015	6.5	43	Valued TIC sectors MD	Acknowlepied	sense recetaled
	PSM0930	2nd		1.11	PT&C	20040019	0.5	20040929	13	50	Two columns terry - no palinity	Acknowleaded	no conductivity
	PSM6933	316	2.2.28 m	ADCP	1450	20041002	12	20050114	8	51			
	P5836930	310	2 2 28 m	ADCP	16xW	20041002	12	20050114	8	-52			
	PSAM933	3d	2228 1	ADCP	MaW	20041002	12	20050114	8	53	Contraction of the second s	1	
	P5006533	3.4			PT&C	20041002	- 12	20050114	0	- 54	Relaty hat computed		
12	P-56J6333	409	6.6.45 1	ADCP	1200	22090114	- 2	20010414	1	35	- 1969 BARRIER - 19	1	
	P-5626933	418	2.2.20	ADCE	14KY	2229901114	- 1	200000011	-4	10			
	P.56,869.10	410	22.00	Mary P	PIAC	20050414	- 10	20050413		53	Last 74b health evaluated		
\$174	P3636331	Tat	2.00	CTD.	TC	20040333	14	20040704	10	59	Regisced by new file hold, 51.04	Replacement	
	P-0836931	Tat.	10 m	CTD	T.C	20040001	- 14	20040700	10	00	Regieved to sew the 2005-03-05	Replacement	
-	PSM6831	1pt	17 m	CTD	T.C	20040001	- 14	20040706	10	-61	Replaced by new fix 2005-23-08	Replacement	
	PSM6931	2nd	2.00	CTD	T,C	20040707	. 18	20040929	9	62			
	PSAJ6931	2nd	10 m	CTD	10	23343737	18	20040929	9	43			
-	PSM6931	2nd	1/ m	CTD	1.0	22040707	78	20040323	- 9	32			
	P-08/6331	20	2.0	CID	1.0	22041001	1	20050111	- 9	22	Part and a State of St.	10.00	Address of the second
	P-0446931	- 22	17.00	CTD.	1.0	22241222		20040111		44	End care a 2004-12-03 - For Blance	2008-02-12	satary mature.
-	P-MAR11	418	6.00	CTD.	TC	23050112	11	20050406	7	44	-		
	P-0446331	115	12 m	CTD	TC	20050112		20050400		73	-	1	
0.00	PSM6831	410	17 m	CTD	T.C	20060112	11	20060406	7	71			
\$4241	PSM8931	1pt	12210	TK.	11x1	22040331	15	20040106	. 9	72			
207.0	P51,16931	2nd	12218	TK	TIXT	20040707	11	20040929	9.5	73			
	P-5636931	- 3e	12210	TK	11x7	20040930	17	20050113	- 9	74	Summer and the second s		
	P-0636531	40		21							Clamaged accurding to plan	-	
\$125	P3M6932	Tat	4 19	RCVI-	UDCTS	23343431	12	20040705	14	75		and the second second	
	-	2nd	4 m	RCM-	U.D.C.T	22043725	17	29040716	19	75	Hary erers Worked only 13-d	Acknowlegded	
	PSM8932	312	4.00	RCM+	UDCT	23063929	17	20050111	14	77	T sensor CK until 2984-12.03 69-38		
_	P.5636932	41	4.18	RUN	00001	173050111	15	20050329	. 7	7.5	page to shired two needs are		
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manne		04	-	ADCO	-	2010141425		200/0124		75	formers bandlet		
-		1 at	-	ALVE		20141214	-	20040704		83	Southern boundary	1	
_	_	Zed		ADCP		20041320	_	20041020		11	horhers boundary	1	
		310	_	1			14		÷.		Purposely demograd due to wanther	1	
		418		ADCP	P	20060413		20060413		12	Aprile's boundary	1	
		418		ADCP	1	20050413		20050413	15	43	Essian boundary		

2 Materials and methods

2.1 Model forcing data – temporal scales

The generic Baltic model (AS3D) employed in this study /Andrejev and Sokolov 1989, 1990/ together with its local variant modelling the Laxemar-Simpevarp area with a horizontal resolution of 0.1×0.1 nautical miles are both based on the primitive (*sensu* fundamental) Navier-Stokes equations formulated on a so-called C-grid /Arakawa 1966/ and is thus inherently similar to many other 3D-models. The numerical implementation has however several advanced features /Andrejev and Sokolov 1997/. The oceanographic state variables are condensed into files that can be inspected and graphically rendered with a specially designed tool named DAS (Data Assimilation System). In the Öregrundsgrepen area earlier development versions of this model have been applied a number of times /Engqvist and Andrejev 1999, 2000, 2008/ and also in special studies with focus on Average Age (*AvA*) and trajectory analysis /Engqvist et al. 2006/ as general measures of water exchange.

An important aspect in the general modelling context is the temporal resolution of the forcing given in Table 2-1. It is seen that the imposed forcing with the highest frequency pertains to the boundary data of salinity, temperature and sea level, which have been computed by the 3D-model of the Baltic. Of these data, the sea level subset is the one with the highest potential to induce rapid changes in the interior of the model domain since such changes are propagated with the speed of a long surface wave, while salinity and temperature fluctuations combine to form density variations which are propagated with the considerably slower speed of internal waves. For the long surface waves it would – under reasonable assumptions – take more than 20 minutes to travel the approximate 15 km from the boundaries to a mid-point of the model area. This in turn means that the shortest expected time-scale of the computed state variables would be of the order of an hour, so this has been the chosen frequency rate at which modelled data have been saved for the ensuing comparison with measurement data.

		data	time re-	Baltic	mode	H (BIS	3D)	Doos	Local	I mode	l (Sin	30)	Remark
Four-law and other model.	data	Ueta	une re-	2004	2004 quar		40	2000	2004	quarte	Late	2005	
Forcing and other model	data	source	seaution	195	ang	ang	411	184	ang	-240	40	191	
Grid of the 3D-modell		NLS	•										
Boundary forcing					<u>├</u>	-	-	\vdash			<u> </u>	\vdash	
Goteborg	cea level	\$MH	1h										1
Skaper	sea level	DMI	1h										1
Laxemar model domain	sea level + S&1		0.5h										Data from the Baltic 3D-model
Meteorological data	nisc. param.	SMH	3h										Mesan data
Freshwater discharge	whole Baltic	ŞMHI	month						-	-			HBV-model data.
-	Laxemarsán	SMHI	W										2005 meas, delivered Mar/05
	Gerseboan	\$MH	W										
Cooling water	volume flow	ONP	month										See Table 5
	over temp.	ONP	-		<u> </u>	<u> </u>	-	-	-	-	-	-	See Table 5
	and-down periods	Contr.	10										See raine 5
Ice formation & breakup			16	-	-	_	_	-					
Initialization S/T data		ICES											Climatic data + spin-up runs
Validation data:				-	<u> </u>	<u> </u>		-	—	-		-	
Sat- & Temp profiles		SMH	1h	L									
Current velocities		SMH	1h	L									
Sea level data		SNH	1h	<u> </u>	<u> </u>	-	-	-		-	-	<u> </u>	
					<u> </u>	-	-	-		-	-	<u> </u>	

Table 2-1. Overview of the forcing and other model data with regard to temporal resolution. ONP stands for Oskarshamn Nuclear Plants, DMI for Danish Meteorological Institute, and NLS denotes National Land Survey of Sweden. Gray fields denote that the data item applies to a particular time period. The assessment of forcing data has not been without problems. The meteorological forcing data (so-called Mueller data set consisting of synoptical geostrophic wind) that have been used in earlier modeling studies /Engqvist and Andrejev 1999, 2000/ were stated by SMHI to be discontinued after 2001. To make up for this loss, so-called Mesan-data were offered to serve as a substitute. The first model runs of 2004 thus relied on the Mesan-data. Late in 2005 it was revealed that the Mueller data set for 2004 was available again and this extension eventually also included the first half year of 2005. A scatter diagram of these two data sets for July 2004 against measured wind speeds at Ölands Norra Udde is presented in Figure 2-1 and yields that the correlation coefficient for the Mesan-data is higher (0.84) than for the Mueller data (0.77), which is the reason for having chosen to use the former data consistently.

Freshwater discharge data with weekly resolution of the two major streams Laxemarsån and Gerseboån have been acquired from SMHI. Both of these streams display a marked seasonal variability, Figure 2-2.

The contemporary operation of the three reactors O1 through O3 requires cooling water which is withdrawn from the coast to the south of these reactors, and after fulfilling its cooling purpose is subsequently discharged with an average excess temperature of about 10°C. However, this cooling water is of no consequence for the advent of a possible leakage of nuclides from a future repository, since when this has been established, the reactors will be shut down according to plan. The cooling water is included in this study because of its factual but rather marginal influence on the water circulation and stratification during the study period April 2004 through April 2005, see Figure 2-3.



Figure 2-1. Comparison of Mueller and Mesan meteorological data relative measured local wind logged at Ölands Norra Udde. The geostrophical Mueller data have been projected to the standard height of 10 m above sea level and have been graphically shifted so that their points do not interfere with the Mesan data. The correlation coefficient of the Mesan data (ρ =0.84) is better than that for Mueller data (ρ =0.77), so the former data set has been used both for the Baltic and the fine-resoution local 3D-model.



Figure 2-2. Freshwater discharge of the two major local streams that discharge into the interior of the local model area. The combined average discharge over the entire validation period amounts to about $0.5 \text{ m}^3\text{s}^{-1}$. The transition between 2004/2005 is shown with a dotted line.



Figure 2-3. Snapshot of the surface temperature in winter conditions of the thermal plume discharge with an excess temperature between 10 and 11°C with a combined flow rate of about 90 m^3s^{-1} (Table 2-2). The three inlets are separately located south of the discharge point and on the shown occasion there is little evidence of recirculation.

Cooling water data have been obtained from the operators of the three nuclear plants. During the model period (April 2004 through April 2005) the discharge of O1 and O2 has been 20 and 25 $[m^3/s]$ respectively, while for O3 the flow rate amounts to 45 $[m^3/s]$. O1 was shut down during most of May 2004 and O2 during August same year, while the non-operational period of O3 mainly coincided with the month of July 2004, see Table 2-2. An indication of the outlet point of the cooling water can be seen in Figure 2-3.

It has not been possible to obtain any reliable ice observations for the coastal waters of the Laxemar-Simpevarp area most likely due to the fact that the comprised winter periods were mild and the coldest period with freezing air temperatures came late in the season (March 2004) and did not last more than a couple of weeks.

2.2 Extraction of model data

For the three stations located on the northern, eastern and southern boundary of the FR-model area encompassing both the data of the Baltic model CR-model code variant (BIS3D) and the local area FR-model (Sim3D) have been saved and made available. (The specific actual program versions are given in Table 2-3). For obvious reasons these data sets should not differ greatly since the latter is derived from interpolated data of the former, notwithstanding that the local FR-model boundary data are also to some degree modified by the interior dynamics of FR-model and the formulation of the boundary conditions. For these boundary stations the Baltic CR-model data have been used as a basis for comparison. For the other locations, that are interior in the FR-domain, the closest equivalent grid cell – both horizontally and vertically – has been chosen. The bulk of work has thus consisted of rearranging the output data of the models into appropriately formatted files suitable for statistical analysis.

	Volume	Over	Not in	Intake	point	5	Disc	harge	point:	
	flux	temp	operation							
Simpevarp 2004:	[m3/s]	[deg. C]	YYYMMDD dates	i	j	depth	i	j	direction	depth
reactors										
01	20	10	040701-040815	47	46	surface	52	49	E	surface
02	25	11	040815-040916	49	46	surface	52	49	E	surface
03	45	11	040522-040612	51	45	bottom	52	49	E	surface

Table 2-2. Overview of nuclear reactor data and their implementation in the FR-model. The letters 'i' and 'j' denote E/W- and N/S-grid coordinates respectively in this local model.

Table 2-3. Correlation coefficients between measured and modelled data, averaged over all measurement periods with valid data taken together. Grey fields mean 'not applicable'. The actual program version of the CR(FR)-model is 'Bis3D1u4'('Sim3D4f3') and the CDB-model version is 'LaxBa25b'. Gray fields indicate 'not applicable'.

		Salinity		Temperatu	ire	U-compone	ent	V-compone	Model	
Station	depth	corr coef	N-	type						
Si21	2.0 m	0.78	259	0.95	325	0.30	693	0.16	693	CR
	10 m	0.77	259	0.93	325	-0.08	693	0.44	693	CR
	17 m	0.90	162	0.82	228	0.01	693	0.44	693	CR
	30 m	0.73	196	0.60	257	0.27	693	0.21	693	CR
SI22	58 m	0.78	187	0.90	187	0.05	374	-0.01	374	CR
Si23	2-20 m					0.10	684	0.01	685	CR
Si24	2 & 5 m	0.80	327	0.94	327					FR
	10 m	0.69	269	0.92	327					FR
	17 m	0.77	327	0.85	327					FR
Si24T	1-21 m			0.84	266					FR
Si25	4.5 m	0.94	3202	0.97	3202	0.49	6510			CDB

2.3 Extraction of measurement data

Initially the extraction of the measurement data was hampered by the things that make data processing difficult: format changes, unmotivated change of units, data without specification, data with erroneous specification, varying depth ranges, transient data retained at the beginning and ending of a measurement period, etc. Most of these nuisances were mitigated for the data files that were submitted into the SICADA database from which the measurement data could be retrieved in a standard format. The naming of the files is given in Table 1-2, and the time of deployment and remarks in Table 1-3.

2.4 Spectral analysis and choice of comparison time frames

In order to find an appropriate sampling rate for making the comparison with simulated salinity and temperature data without missing relevant variations and thereby producing bias (so-called *alias* errors), the power spectra for representative months of the different seasons have been investigated using the Fast Fourier Transform (FFT) in the Matlab toolbox. The typical outcome of this encompassing analysis is presented in Figure 2-4 concerning temperature and Figure 2-5 for salinity, from which it is clear that the bulk of the contained variance concerning salinity and temperature measurements is located in the part of the spectra that lies below diurnal rates, i.e. once a day. Thus daily samples of measured and simulated salinity and temperature can be compared without loss of generality and introduction of spectral aliases.



Figure 2-4. Temperature spectra of station Si21 with regard to depth and seasonality. Each of the 16 'subplots' is a so-called power spectrum and its y-axis thus denotes the variance distribution with regard to sampling frequency of the temperature measurements. Combinations with missing data are left empty. With the possible exception of August and 17-m depth, most variance is located at frequencies below 1 day⁻¹. This means that the comparisons to simulated data can be performed with daily samples, which frequency is indicated with a red dotted line.



Figure 2-5. Salinity spectra of station Si21 with regard to depth and seasonality. Each of the 16 'subplots' is a so-called power spectrum and its y-axis thus denotes the variance distribution with regard to sampling frequency of the salinity measurements. Combinations with missing data are left empty. Without exception all variance is located on frequencies above 1 day⁻¹. This means that the comparisons to simulated data can be performed with daily samples, which frequency is indicated with a red dotted line.

In Figure 2-6 the corresponding spectrum analysis is performed on the ADCP instrument placed at station Si21 where 19 layers of orthogonal current components are measured. Both panels pertain to period 1 and span the depth interval 3 m through 39 m. The east/west (U) current component displays more variance for frequencies higher than 2 day⁻¹ (i.e. twice a day), than the north/south (V) current component, but even for the bottom layers most of the variance is found below this frequency. This means that semidiurnal sampling suffices to give a fair comparison to simulated data. To be on the safe side all current comparisons have been conducted with a semidiurnal (12 h) sampling rate. This also applies to most of the current measurements at other locations.



Figure 2-6. a (left panel). The spectra of the east/west(U)-velocity components. Each of these 19 'subplots' is a so-called power spectrum with its y-axis thus denoting the variance distribution with regard to the frequency of the measured velocity's U-component, which shows that most variance is located below the frequency 2 day⁻¹ i.e. twice a day. b (right panel). The spectra of the north/south(V)-velocity components. Each of these 19 'subplots' denotes the same the variance distribution as for figure a, but with regard to the frequency of the measured velocity's V-component. Virtually all variance is located at frequencies below once a day or equivently with a diurnal periodicity. For all subplots in both panels this diurnal periodicity is indicated with a red dotted line.

2.5 Statistical methods of comparison

The method of comparison is direct and straightforward. The corresponding data as to horizontal and vertical location are extracted with their FFT-determined appropriate sampling rates and are subsequently subjected to ocular and statistical comparison. The latter consists of invoking the cross-correlation function that is supplied in the Matlab toolbox together with graphically depicted regression lines. All computed correlation coefficients are summarized and accounted for in Table 2-3. It can be pointed out that concerning the regression lines, the slopes are often less than unity, which value corresponds to a hypothetical perfect match between the data set pairs. Inaccuracy in the measurements can be shown to significantly contribute to such less-than-ideal slopes (Anders Grimvall, pers comm).

3 Results

3.1 Overview and intercomparison of salinity and temperature measurements

First an overview of the scalar measurement entities salinity and temperature is given in Figure 3-1. The most striking feature is the noticeable fluctuation of salinity measured at station Si22 in the depth bracket around 50 m. Some tendencies towards unstable stratification (water with higher salinities on top of deeper layers at approximately the same temperature) can be observed, for example at Si24. This will be scrutinized more in detail when the data of the separate station are analyzed below. At station Si23 only velocity was measured. The intercomparison of salinity and temperature measurements between the stations seems otherwise consistent within the allowance that the data gaps necessitate. The salinity and temperature levels are seemingly comparable between the stations. At station Si24 temperature was also measured with a thermistor chain with eleven levels giving an improved vertical resolution. This will be examined in detail below.



Figure 3-1. Overview of the salinity and temperature measurements of all stations at which these scalar entities were measured. The overall signatures of different stations are strikingly similar with the exception of Si22 that is measured at a considerably deeper depths of about 50 m. This station displays a conspicuously extended leading data gap. Data gaps of other stations may not be as easily identified in this figure since curves may overlap. Obviously erroneous data can in spite of this be seen for Si25. At the station Si23 only velocities were measured and this station has thus been exempted from this overview.

3.2 Station Si21

At the peripheral station Si21 positioned near the center of the northern boundary all four parameters (salinity, temperature and two orthogonal velocity components) were logged. A closer look at the salinity and temperature curves pertaining to Si21 in Figure 3-1 reveals that the salinity stratification (upper panel in Figure 3-2) is seemingly stable, while in autumn penetrative convection makes the salinity curves almost coincidental. The vertical line at the onset and termination of each measurement period help to identify the transitions between the four measurement periods. These endpoints have systematically been removed in the ensuing statistical analysis and this applies to the time series of all stations.

The temperature measurements (lower panel in Figure 3-2) made during the spring and summer heating period (before JD 225) are due to the formation of a thermocline, only occasionally interrupted by vertical mixing and possible up-/down-welling events that only affect the two surface-most measurement depths, e.g. near JD 160. The same consistency applies to the cooling period (after JD 300) when thermally well-mixed conditions mainly prevail from the 2- to 30-m depth. The noticeable continued cooling at the 30-m level during the first period is probably due to an onset of the same instrument malfunctioning that disqualified its data during the second period.

Such vertical mixing events represent an irreversible and thus lasting effect. A wind-induced down-welling, on the other hand, means a temporary vertical redistribution of water which should recoil quite soon after the wind subsides. This has little lasting effect on the internal vertical distribution of the salinity and temperature fields.



Figure 3-2. Overview of the salinity and temperature measurements at Si21. The salinity stratification is seemingly stable and the temperature curves are consistent with springtime formation of a thermocline, while in autumn penetrative convection makes both the salinity and the temperature curves almost coinciding. The vertical part on the onset and termination of each respective measurement period helps to identify the transitions between the four measurement periods.

In Figure 3-3 the temperature development during the entire validation period is shown with measurements at the respective depth layers together with the corresponding simulated values. With the exception of the measurement at 30 m that was discontinued about JD 200, the transitions between the measurement periods are clearly visible. The surface-most measurements and simulated temperature curve match one another quite well. Also at the rapid cooling instance about JD 320–350 there is an almost exact match between observed and modeled temperatures at all four depths.

Simulated and observed salinities at station Si21 for the duration of the validation period are depicted in Figure 3-4. In addition to a general falling trend of the simulated salinity curves, there are both similarities and differences. In spite of the noticeable offset for the curve pairs for the depths between 2-m and 17-m until JD 300, these pairs are obviously strongly covariant, which is most clearly seen at the salinity depletion event occurring on JD 200 through 240. At the end of the entire simulation period all curves converge.

In Figure 3-5, the scatter diagram displays differences between measured and simulated temperatures at station Si21. The corresponding correlation coefficients are given in Table 2-3 and amounts to 0.95 for the surface layer but diminish to 0.60 at 30 m.

A scatter diagram between measured and simulated salinities of the station Si21 is displayed in Figure 3-6 with separate regression lines for the four depths. The corresponding correlation coefficients are given in Table 2-3 and are on the 0.80 level, which means that most of the measured salinity dynamics (64%) is captured by the model. The regression lines for the surface measurements are closer to the ideal diagonal line, and for all four depths the slope of the regression lines is close to the ideal 1:1 slope.



Figure 3-3. Comparison of simulated (dotted) and measured (solid) temperature data for different depths at station Si21. With the exception of the measurement at 30 m that was discontinued about JD 200, the transitions between the measurement periods are clearly visible. The surface-most measurements and simulated temperature curve match one another quite well. Also at the rapid cooling instance about JD 320 there is an almost exact match between all four pairs of curves.



Figure 3-4. Comparison of simulated (dotted) and measured (solid) salinity data for different depths at station Si21. In spite of the noticeable offset between the measured and the simulated values until JD 300, these pairs are obviously strongly covariant, which is most clearly seen at the salinity depletion event occurring on JD 200 through 240. At the end of the entire simulation period all time series come closer together.



Figure 3-5. Scatter diagram for measured and simulated temperature of Si21 with regression lines for the four depths in same colors as is indicated by the legend. The line that indicates a perfect match is depicted in black. The corresponding correlation coefficients are given in Table 2-3 and are 0.95 for the surface layer but diminish to 0.60 at 30 m which is to some extent a consequence of the restricted range of the temperature variation over the year cycle at this depth. The regression lines are quite close to the ideal line in black.



Figure 3-6. Scatter diagram for measured and simulated salinity of Si21 with regression lines for the four depths in same colors as is indicated by the legend. The line that indicates a perfect match is depicted in black. The corresponding correlation coefficients are given in Table 2-3 and are on the 0.80 level which is a reassuring expression that most of the measured dynamics is captured by the CR-model. The regression lines for the surface measurements are closer to the ideal line, and for all four depths the slope of the regression lines is close to the ideal.

In Figure 3-7 contour diagrams of measured E/W-velocity (U-) component at station Si21 are depicted with a half-hour sampling rate but processed with a 5 h-running average filter and compared to the correspondingly processed simulated data. The measurements were conducted with an ADCP instrument. There are no striking similarities of the features of these diagrams. The current levels are basically comparable, with only a few notable exceptions. The overall correlation levels are in spite of this comparatively high for the surface and the bottom measurements, see Table 2-3. This figure foremost confirms the apprehended considerable temporal variance in the flow field.

Contour diagrams of measured N/S-velocity (V-) component at station Si21 are shown in Figure 3-8. These diagrams are based on the same sampling rate as in Figure 3-7, i.e. smoothed with a 5 h running average filter and compared to the correspondingly treated simulated data. The current levels are basically comparable with only a few notable exceptions. On JD 350–380 the simulation shows an intensification of current from the surface to the bottom that has no counterpart in the measured data. In spite of this for the two intermediary levels the correlation coefficients are 0.44 (Table 2-3).

In Figure 3-9 a scatter plot between measured and simulated N/S-current velocity (V-component) velocity of Si21 is given. Ocular inspection gives that there is only a faint, if any, tendency of alignment along the ideal diagonal, but the range of the two data sets is the same. The correlation coefficients are given in Table 2-3 for the computed depths that are closest to the measured depths.

Correlation between measured and simulated E/W- current velocity (U-) component velocity of Si21 is shown in Figure 3-10. In comparison to Figure 3-9, ocular inspection shows even less tendency of alignment along the ideal diagonal. The correlation coefficients are given in Table 2-3 and are highest for the top and bottom levels 2 m and 30 m, i.e. complementary to the levels of the maxima found for the N/S-component.

Common to both these velocity correlation diagrams is that the simulated data range is comparable to the measured data range.

In Figure 3-11 a comparison of current speed spectra for six depth levels is presented. The frequency distribution of the variance of the measured and simulated data is similar despite that the found correlation coefficients are quite small and even negative in a few instances. For the surface-most layer there is unevenly distributed variance over the entire frequency range that does not correspond to the simulated data. For the 5 m-layer there is coinciding variance for the frequency around 0.3 day^{-1} . For all spectra of the simulated currents, the major variance is found at frequencies lower than about 0.1 day^{-1} .



Figure 3-7. Contour diagram comparison between measured and simulated E/W-velocity (U-) component of Si21. In order to enhance any similar features these data series have been processed with a 5 h-running average filter. The measurements were conducted with an ADCP instrument. Periods with no data are blanked. There are no striking similarities of the features of these diagrams. The current levels are basically comparable with only a few notable exceptions. The overall correlation levels are, in spite of this, comparatively high for the surface and the bottom measurements, see Table 2-3.



Figure 3-8. Contour diagram comparison between measured and simulated N/S-velocity (V-) component of Si21. The comparison is based on a 0.5-h sampling rate but processed with a 5 h-running average filter. Periods with no data are blanked. The current levels are basically comparable with only a few notable exceptions. On JD 350–380 the simulation shows an intensification of current from surface to the bottom that has no counterpart in the measured data. For the two intermediary levels the correlation coefficients are 0.44 (Table 2-3).



Figure 3-9. Correlation between measured and simulated N/S- current velocity (V)-component velocity of Si21. Ocular inspection may suggest that there is a slight tendency of alignment along the diagonal. The correlation coefficients are given in Table 2-3 and are highest for the intermediary levels 10 m and 17 m.



Figure 3-10. Correlation between measured and simulated E/W- current velocity (U)-component velocity of Si21. Ocular inspection does hardly indicate any tendency of alignment along the diagonal. The correlation coefficients are given in Table 2-3 and are highest for the top and bottom levels 2 m and 30 m, i.e. complementary to the levels of the maxima found for the N/S-component.



Figure 3-11. Comparison between measured and simulated velocity spectra of station Si21. For the surface-most layer there is unevenly distributed variance over the entire frequency range that does not correspond to the simulated data. For the 5-m layer there is coinciding variance for the frequency around 0.3 day⁻¹. For all spectra of the simulated currents, the major variance is found at frequencies lower than 0.1 day⁻¹.

3.3 Station Si22

The measurement data of station Si22 only exist for the third and fourth periods due to instrument failure. During these periods the instrument was dislocated due to interference by ships so that different depths are indicated for the two measurement periods: 58 m (49 m) for the third (fourth) period.

An overview of the salinity and temperature measurements for these two periods is given in Figure 3-12. In spite of the changed measuring depth, both the salinity and the temperature curves are continuous with no obvious jump indicating the transition between the third and the fourth periods. The time when the instrument was inadvertently dislodged has not been possible to establish. To complicate matters further, a second instrument was deployed at Si22 (Table 1-3) but only functioned five days and gave no salinity recordings.

The salinity spiked several times during these two periods but resumed an average interval between 7 and 8 psu. The temperature curve displays an almost monotonous seasonal decline during winter and then rises slightly toward spring which is consistent with the damping of the seasonal surface signal with depths.

A comparison of the measured and simulated temperature at these depths at station Si22 is shown in Figure 3-13. After JD 380 the two curves are obviously quite covariant. Prior to this date there are at least similar levels but the measurements display more rapid transitions that the simulated time series do not capture.



Figure 3-12. Overview of salinity and temperature measurements at station Si22. Only in the third and fourth measurement periods was this instrument in proper operation. It was further accidentally dislodged from its original placement so that different depths are indicated for the two measurement periods: 58 m for the third period and 49 m for the fourth.



Figure 3-13. Comparison of measured and simulated temperatures at station Si22, with the transition between 2004/2005 indicated by a broken line. At least during 2005, the covariation between the measured and the simulated data is strikingly good which is confirmed by the correlation level given in Table 2-3.

The corresponding diagram concerning salinity (Figure 3-14) shows that the transition events are almost simultaneous but that the simulated curve does not reach the same amplitudes as does the measured curve, even though the levels are comparable.

In Figure 3-15 a scatter diagram of measured versus simulated temperature at station Si22 is shown. The simulated temperatures are slightly overestimated but the slope of the regression line is acceptably close to the 1:1 slope of the ideal line. The correlation coefficient is 0.90.

The corresponding scatter diagram (Figure 3-16) for salinity displays a regression line that slopes considerably less steeply than an ideal relationship. This could partly be caused by the two different depths that were involved. The correlation coefficient is 0.78.

A comparison of E/W-component of the current at Si22 shows (Figure 3-17) that the measured current component flows steadily to the east while the simulated current reverses direction a number of times. The current intensities are however comparable. The corresponding comparison of the N/S-component (Figure 3-18) shows that there is almost no flow in this direction. The most likely explanation is that the instrument during both periods had been inadvertently deployed in a rift oriented in the E/W-direction.

Scatter diagrams of the east/west(U)- and north/south(V)-velocity components at station Si22 at 12-m depth are given in Figure 3-19 and Figure 3-20 respectively. The corresponding small correlation coefficients (Table 2-3) confirm what an ocular inspection already has made obvious.

In Figure 3-21 a spectral comparison of the simulated and measured current speed at station Si22 is presented. This comparison is independent of the current direction and demonstrates that the spectral appearances are not notably dissimilar in spite of the small correlation coefficients of the U- and V-velocity components, although the measurement data have more variance located towards higher frequencies.



Figure 3-14. Comparison of the measured and simulated salinity at station Si22. After JD 350 the covariation between the measured and the simulated data is seemingly good which is confirmed by the comparatively high correlation given in Table 2-3. During the period JD 350–390 both the measurement and the simulated data make a simultaneous jump upward even though the measurement time series reaches higher values than the modeled data.



Figure 3-15. Scatter diagram for measured and simulated temperature of Si21. The green diagonal line represents the ideal relationship. The black line is a regression line, the slope of which is acceptably close to the green diagonal line.



Figure 3-16. Scatter diagram for measured and simulated temperature of Si21. The green diagonal line represents the ideal relationship. The black line is a regression line, the slope of which is considerably less steep than the ideal diagonal (green) line. This could at least partly be explained by the two different depths on which the instrument was deployed during the third and fourth periods. The time when the instrument was accidentally dislodged is not possible to establish.



Figure 3-17. Comparison between measured and simulated E/W-velocity (U-) component of Si22. Data are available only for the two last measurement periods. Virtually no correlation can be visually discerned which is also confirmed in Table 2-3.



Figure 3-18. Comparison between measured and simulated N/S-velocity (V-) component at station Si22. Data are available only for the two last measurement periods starting on JD 300. Virtually no correlation can be visually discerned which is also confirmed in Table 2-3.



Figure 3-19. Scatter diagram for measured and simulated E/W-velocity (U-) component of Si22. This pattern seems like a rectangular distribution and yields a correlation coefficient of a mere 0.05 according to Table 2-3.



Figure 3-20. Scatter diagram for measured and simulated N/S-velocity (V-) component of Si22. The lack of variation in the measured data is most likely due to an accidental placement of the instrument in a rift that is oriented in the orthogonal (E/W) direction.



Figure 3-21. Comparison between measured and simulated velocity spectra of Si22. Both spectra display variance contribution distributed over the entire range down to the Nyquist frequency (once per day) but the measurement data have more variance located towards higher frequencies. The measured data are unknown as to their depth that could be somewhere between 49 m to 58. The compared simulated data are taken from the layer centered about 40 m depth.

3.4 Station Si23

At station Si23 only ADCP-measurements were made. In Figure 3-22 a contour diagram comparison between measured and simulated E/W-velocity components is presented. In order to enhance any similar features, these data series have been processed with a 5 h running average filter. The current levels are basically comparable with only a few notable exceptions, in particular for the surface-most layers.

Corresponding contour diagram comparison of the N/S-velocity component between measured and simulated currents is shown in Figure 3-23. The current levels are again comparable with some exceptions for the surface-most layers.

Scatter diagrams between measured and simulated E/W (N/S)-components of velocity at Si23 are presented in Figure 3-24 (Figure 3-25). No correlation is visually discernible, and the average correlation coefficient over the entire water column amounts to 0.1 (0.01) according to Table 2-3.

In Figure 3-26 a comparison is shown between measured and simulated velocity spectra at Si23. With the exception of the 10-m level, most measured variance is found for frequencies below 0.1 day⁻¹. This feature is also regenerated by the simulated data, but with a small contribution to the surface-most layer for daily variations.



Figure 3-22. Contour diagram comparison between measured and simulated E/W-velocity (U-) component of Si23. Periods with no data are blanked. In order to enhance any similar features these data series have been processed with a 5 h-running average filter. The measurements were conducted with an ADCP instrument. The current levels are basically comparable with only the notable exception for the surfacemost layers JD 100-180. The overall correlation level averaged over the water column amounts to 0.1, see Table 2-3.



Figure 3-23. Contour diagram comparison between measured and simulated N/S-velocity (V-) component of Si23. Periods with no data are blanked. In order to enhance any similar features, these data series have been processed with a 5 h-running average filter. The measurements were conducted with an ADCP instrument. The magnitudes of the current levels are basically comparable but otherwise there is virtually no agreement between these two contour plots. The overall correlation level averaged over the water column amounts to a mere 0.01, see Table 2-3.



Figure 3-24. Scatter diagram for measured and simulated velocity (*E/W*-component) at the station Si23. No correlation pattern is visually discernable, and the average correlation coefficient over the entire water column amounts to 0.1 according to Table 2-3.



Figure 3-25. Scatter diagram for measured and simulated velocity (N/S-component) at the station Si23. No correlation pattern is visually discernable, and virtually no correlation exists between these time series. The overall correlation level averaged over the water column amounts to a mere 0.01, see Table 2-3.



Figure 3-26. Comparison between measured and simulated velocity spectra of Si23. With the exception of the 10-m level most measured variance is found for frequencies below the 0.1 day^{-1} limit. This feature is also regenerated for the simulated data with a small variance contribution towards the surface-most layer for daily variations.

3.5 Station Si24

The placement of this station (Si24) in the interior of the computational domain of the FR-grid is intended to make it possible to validate to what extent the imposed forcing via the boundaries is propagated and reflected in the interior of the local model grid. All three previous station (Si21 through Si23) have been validated against computed data of the Baltic (CR-) model.

First an overview of the salinity and temperature measurements is given in Figure 3-27. The salinity curves indicate stable stratification during the two first measurement periods, but then the 10-m curve deviates more than what is acceptable according to the stipulated inaccuracy of \pm 0.1 units in the psu-scale /Johansson and Morosini 2002/. The temperature curves are consistent with springtime formation of a thermocline, while in autumn penetrative convection makes both the salinity and the temperature curves almost coincidental.

The comparison of measured and simulated temperature curves in Figure 3-28 shows that the events of rapid heating and cooling transitions are strikingly coincidental but not always on the same temperature level. For the 17-m data around JD 250 the levels also coincide in a satisfactory manner. The temperature levels of the rapid heating and cooling instances appear fully consistent which is substantiated by the corresponding correlation coefficients given in Table 2-3. These diminish slightly towards the bottom-most layer (17 m), but as an average still stay over 0.9.



Figure 3-27. Overview of the salinity and temperature measurements at Si24. The four measurement periods are easily identified by the 17-m curve going down to the x-axis. The salinity stratification is seemingly stable with the exception of the 10-m curve during the third measurement period (JD 290–240) and the entire fourth period. The temperature curves are consistent with springtime formation of a thermocline, while in autumn penetrative convection makes both the salinity and the temperature curves almost coincidental.



Figure 3-28. Comparison of measured (solid lines) and simulated (broken lines) temperature at station Si24. The levels and heating and cooling instances appear show a good agreement which is substantiated by the corresponding correlation coefficients given in Table 2-3.

The comparison of measured and simulated salinities, depicted in Figure 3-29, shows that at the onset of the measurement period on JD 100, the model produces a distinct salinity stratification whereas the measurements show no such stratification. This difference is most likely a consequence of the initialization procedure that in absence of measurement data must resort to reiterated runs with climatologically based forcing. During measurement periods two and three the measured and simulated salinities converge with only a few more instances of elevated values for the bottom-most layer (17 m). The unstable stratification for the measured 10-m data is conspicuous. With these data exempted from the computations, the correlation coefficients fall nevertheless as an average in the range 0.7–0.8, see Table 2-3.

A scatter diagram between measured and simulated temperature data for Si24 is presented in Figure 3-30. The regression line of the surface-most layer coincides well with the ideal line and the corresponding regression lines of the other two depths display that the model slightly under(over)estimates the measured data for temperatures above(below) about 7°C.

The corresponding scatter diagram between measured and simulated salinity data for Si24 in Figure 3-31 also shows satisfactory correlation levels as for the temperature. The regression line of the surface-most layer coincides almost perfectly with the ideal line with only a slight systematic underrepresentation. The corresponding bottom-most layer, on the other hand, systematically over-represents with the same amount. Their slopes are well aligned with an ideal 1:1 slope. The 10-m regression line falls between the regression lines of the two adjacent layers.

The good agreement between measured and simulated temperature and salinity data that are computed for an interior point of the local FR-model evidently vouch for the fully acceptable realism and the precision of this model approach concerning its capacity to simulate the variability of these fields in the interior of the FR-model domain.

At station Si24T the temperature measurement was also complemented by a thermistor chain with eleven sensors that covered the depth range from 1 m to 21 m. According to plan this was deployed during the three first measurement periods. The formation of temporary thermoclines and their resolution by the autumnal penetrative cooling process can be clearly seen in Figure 3-32. The FR-model underestimates the heat penetration but the overall similarity is quite satisfactory.

This is substantiated by the scatter diagram (Figure 3-33) between measured and simulated temperature data for station Si24T. The comparison is made for the measurement levels that coincide closest to the layer partitioning of the numerical model. The regression line of the surface-most layers coincides well with the ideal line in solid black and the corresponding lines of the other three depths are also quite satisfactory, even though their slopes diminish somewhat towards the bottom.



Figure 3-29. Comparison of measured (solid lines) and simulated (broken lines) salinity at station Si24. At the onset of the measurement period on JD 100 the simulated data show a weak salinity stratification whereas the measurements indicate mainly vertically homogeneous conditions. This difference is probably a consequence of the initialization method. During measurement periods two and three the measured and simulated salinities converge with only a few more instances of elevated values for the bottom-most layer (17 m). The unstable stratification period for the measured 10-m data (JD 290–340) is quite conspicuous and has been exempted from the correlation coefficient computation.



Figure 3-30. Scatter diagram for measured and simulated temperature data for Si24. The regression line of the surface-most layer coincides almost perfectly with the ideal line in solid black and the corresponding lines of the other two depths are also quite satisfactory. The correlation coefficients diminish slightly towards the bottom-most layer of 17m but their average still stays over 0.9.



Figure 3-31. Scatter diagram of measured and simulated salinity data for Si24. The regression line of the surface-most layer coincides well with the ideal line in solid black with only a slight systematic under-representation of about 0.1 psu. The corresponding bottom-most layer on the other hand systematically over-represents with the same amount. All three regression lines have close to an ideal 1:1 slope. The 10-m regression line is only slightly misaligned and falls in between the regression lines of the two adjacent layers. The correlations fall in the range 0.7-0.8 (Table 2-3).



Figure 3-32. Comparison between measured and simulated temperature of Si24T. The measurements were performed with a thermistor chain and the transition between the three measurement periods can be seen as black/gray vertical stripes. The formation of temporary thermoclines and their resolution by the autumnal penetrative cooling process can be clearly seen. The model evidently underestimates the heat penetration but the overall similarity is satisfactory. The white color for the simulated temperatures denotes temperatures between zero and the freezing point of the local sea water about -0.3° C.



Figure 3-33. Scatter diagram of measured and simulated temperature data for Si24T, employing a thermistor chain. The comparison is made for the levels that coincide closest with the layer partitioning of the numerical model. The regression line of the surface-most layers coincides well with the ideal line in solid black and the corresponding lines of the other three depths are also quite satisfactory, even though their slopes diminish towards the bottom.

3.6 Station Si25

Figure 3-34 gives an overview of the salinity and temperature measurements at station Si25. At this station these two scalar variables were measured together with the velocity by an instrument deployed near the bottom of the channel-like western part of the elongated major entrance basin Djupesund that connects the interior basins around the Aspö island with the sea (Figure 3-35). For these secluded land-locked basins the local 3D-model must be regarded as inappropriate with regard to realism, foremost because the bathymetrical features cannot be resolved with the resolution set by other considerations. Instead the CDB-model was formulated to this end. This has been developed in stages since it was first applied to the basins adjacent to the Äspö island /Engqvist 1997/. Its present enhanced features have been described in /Engqvist and Stenström 2004/ and it has been successfully validated in the Himmerfjärden area 40 km south of Stockholm /Engqvist and Stenström 2008/. Its adaption to the present task is given in Figure 3-35a. Since Djupesund is considered to be a basin, the corresponding comparison between measured and simulated data is made at the strait S3 connecting the sub-basin Djupesund (SB24) to Kalvholmsfjärden (SB21). For these sub-basins the partitioning is based on strict coastal oceanographic considerations. The accounting of water exchange from an ecological point of view may not need this level of detail. A few basins have thus been conjoined and then given a separate name when passing on the computation results to the ecological modeling group.

The surface heat exchange with the atmosphere for this CDB-model is driven by measurements in the surface layers of Granholmsfjärden and Borholmsfjärden. These measurements compare favorably (Figure 3-36) with modelled surface temperature at the point named R-1 in Figure 3-35a, located about 1 km off the coast. The simulated salinity and temperature profiles at this station are used as boundary forcing for the CDB-model.



Figure 3-34. Overview of salinity and temperature measurements at the station Si25. Both salinity and temperature measurements during period two are missing and the temperature data for period three are obviously erroneous.



Figure 3-35. a (upper panel). Stylized block diagram rendering the naming of the sub-basins (SBs) with blue labels (and the straits with red labels) employed in the CDB-model. Basin labels in bold refer to the ones that are accounted for in related ecological analysis. b (lower panel). The partitioning of the Laxemar coastal area into sub-basins. The locations for which the density profiles computed by the 3D-model are used to force the CDB-model have been indicated by R-1 and R-2. The approximate location of stations Si24 and Si25 in Djupesund have been indicated by a black dot and a red circle respectively (excerpt from bassangindelning_20050926_1400.mxd).



Figure 3-36. Measured surface temperatures of the inner Laxemar-Simpevarp basins used for forcing of the CDB-model. The average temperature of the Granholms- and Borholmsfjärden are used for all the modeled SBs, while the costal station data apply to R-1 and R-2.

For the sea-level forcing the simulated sea level at R-1 could have been used, but this would mean that deviations introduced by the FR-model would have added to the inherent uncertainties of the CDB-model. In order to give the CDB-model as fair individual validation as possible, it was decided to use measured sea level data which exist for most of the validation periods at a local station (PSM000371), complemented with about one month (April) of measurements at a more distant gauge station (Oskarshamn), see Figure 3-37. A scatter diagram of the hourly measured sea levels during the overlapping month of May is depicted in Figure 3-38 with a correlation coefficient of 0.93 (N=97), which gives reassuring evidence that this procedure is sound.

Together with the wind data set logged at Ölands Norra Udde (Figure 2-1) and the freshwater discharge of Laxemarsån (Figure 2-2), the CDB-model forcing is accounted for.

A first comparison between modeled and measured salinity and temperature data at station Si25 is shown in Figure 3-39. In addition to the data gap in the second period, there are two shorter periods for which the salinity measurements are obviously erroneous. For the temperature measurements also the third measurement period must be discarded. For the remaining time periods the measurement data generally display a more ragged appearance than the simulated data. This is a consequence of the CDB-model's instantaneous horizontal mixing that precludes the model from upholding the same gradient as the measured differences between the concentrations on the up- and down-estuary sides of the strait.

The correlation between measured and simulated temperatures can be seen from the scatter diagram in Figure 3-40. On average the simulated data underestimate the measured. In spite of the data gaps the correlation coefficient is 0.97.

The corresponding scatter plot between measured and simulated salinity data is shown in Figure 3-41. Since the measured data are split into two periods with differing levels of salinity, this means that the scatter plot shows two isolated clusters. The correlation coefficient of either group is about 0.5 and the one of the conjoined groups encompassing the entire data set amounts to 0.94, which elevated value should be regarded more as a reflection of the bi-modal distribution than as a virtue of the model.

The deployment of the current measurement to a channel reduces to a large extent the degrees of freedom since the current will mainly be constrained to flow in the channel direction. In Figure 3-42 a comparison of the simulated and the measured along-channel current speed at a level near the bottom is presented. It is evident that the current intensities are comparable in spite of possible misrepresentation of the section area at the level of the actual instrument placement. The correlation diagram in Figure 3-43 shows that the intersection point between the regression and the ideal lines is close to the point representing zero velocities for both axes. The difference in slope can thus be attributed to the above-mentioned difference in cross-section area. The correlation coefficient is 0.49 which according to Table 2-3, is in par with the highest correlation levels achieved with the 3D-model.

The corresponding comparison of the spectra of the simulated and measured velocity data can be seen in Figure 3-44. Since the measurements were performed with a temporal resolution of one hour, the Nyquist frequency is 12 day⁻¹, though the CDB-model was run with a comparatively shorter time step.



Figure 3-37. Sea-level forcing of the DB-model. The first part (red line) covers the time period January through May 2004 and is measured by SMHI at their Oskarshamn station. The second part (blue line) is from local measurements at the SKB-site PSM000371 and covers May 2004 through March 2005. Thus there is a one-month overlap of these data sets which makes the scatter diagram in Figure 3-38 possible.



Figure 3-38. Scatter diagram of the overlap period (May 2004) for the two sea level data sets used. Some points may be coinciding due to the limited numerical resolution. The correlation coefficient is ρ =0.93 (N=97).



Figure 3-39. Overview of measured and simulated salinity and temperature data of Si25. The data are obviously erroneous for both measurement series during measurement period two and for the entire period three regarding temperature. The measurement data display generally a more ragged appearance due to the greater differences between the concentrations on the up- and down-estuary side of the strait. A 24-h running average has been superposed on the measured data to facilitate comparison.



Figure 3-40. Correlation between measured and simulated temperature of Si25. On average the simulated data underestimate the measured. In spite of the data gaps the correlation coefficient is 0.97.



Figure 3-41. Scatter plot for measured and simulated salinity of Si25. Since the measured data are split into two periods with differing levels of salinity, this means that two isolated groups of point cluster occur. The correlation coefficient of the conjoined groups i.e. ρ =0.94, but for each individual group the correlation level is considerably inferior. For the lower of the two groups representing measurement period one, the simulated data overestimates the measurement data, which in turn has the consequence that the slope of the red regression line entailing all data is smaller than the diagonal line in green.



Figure 3-42. Comparison between measured and simulated current velocity components in the strait direction of Si25. During the fourth measurement period (starting on JD 375) there is a notable change in the current velocity amplitude most likely due to the fact that the instrument was deployed on a deeper location than earlier. Both these data series have been processed with a 24-h running average filter, shown as superposed black curves. Two data items were missing in the measurement file and have been restored by interpolation.



Figure 3-43. Scatter diagram for measured and simulated current velocity component in the strait direction of Si25 with hourly temporal resolution. The regression line in red underestimates the simulated current but this can be explained by differences in the strait section areas that are represented. In the model a larger area is associated with the computed average flow, while the measured current represents just the strata where the instrument is deployed. The correlation coefficient ρ =0.49, see Table 2-3.



Figure 3-44. Comparison of spectra of measured and simulated current velocity component in the strait direction of Si25 for the third measurement period with hourly temporal resolution. Current spectral components exist for higher frequencies than the Nyquist frequency, at least for the simulated data. These spectra have been smoothed with a running average filter and the similarity must be deemed as fully acceptable.

3.7 Transects

Five transects with a ship-mounted ADCP instrument have been performed along parts of the southern, northern and eastern boundaries, Figure 3-45. All these transects were done under sufficiently calm weather conditions and can thus not be considered as representative of the average water circulation along these transects. Figure 3-46 shows the transect along part of the southern boundary 2004-04-28 (JD 119 after 2004-01-01) going westward toward station Si23 but not reaching it. Even though station Si23 falls somewhat to the left of the diagrams, the currents measured by the stationary ADCP instrument data (Figure 3-22) are not inconsistent with these vessel-mounted data. The diagrams span close to two nautical miles and give thus an appreciation of the variability within one grid cell of the Baltic CR-model.

The next transect was taken 2004-07-07 (Figure 3-47) with almost identical starting and ending points as for Figure 3-46, but the surface current direction is reversed and the feeble current of the bottom layer is flowing southward. The horizontal homogeneity of the flow pattern representing one grid cell of the Baltic CR-model is again convincingly apparent. Comparison to the measurements with the stationary ADCP deployed at station Si23 is not easy due to the weak current intensities but no obvious inconsistencies between these measurements can be detected.

The transect along part of the northern boundary 2004-10-20 going westward toward station Si21b (see Figure 3-45) – but not reaching it – is shown in Figure 3-48. The homogeneity of the diagrams that span one grid cell of the Baltic CR-model is fully acceptable even though there is a slight deepening of the surface layer to the east. The date of this transect corresponds to JD 294 in Figures 3-22 and 3-23 and a comparison to these stationary ADCP-measurements is again hampered by the weak current intensities.

In Figure 3-49 is depicted the transect along part of the northern boundary 2005-04-13 going eastward from station Si21b. This date represents the last measurement day. In fact this transect was taken a couple of hours after the stationary ADCP instrument was lifted out of water. In spite of the differing current scale compared to the previous transects, the current magnitude was very weak. Because of this, the heterogeneity displayed for the horizontal layers, shifting from currents setting northward in the right half of the diagram to currents setting west in the left half, can hardly be interpreted as an indication of current features appearing on a sub-grid cell level.

Finally, the transect along part of the eastern boundary on the same date (2005-04-13) as the previous transect going southward passing near station Si22, see Figure 3-50. The vessel-mounted ADCP instrument gives current readings down to about 40 m. Beyond this range, however, only occasional data are given. At the date of this transect, the current meter at Si22 was deployed at a depth of 49 m. This completely dismisses any possibility to compare with the stationary current meter at this station. The current pattern within the two nautical miles covered does not give rise to concern about the horizontal current homogeneity of the Baltic CR-model.



Figure 3-45. Transects along parts of the southern, northern and eastern FR-model boundaries. The starting points are marked as green circles and the end points with a red circle. The FR-model domain is outlined as a light blue rectangle with measurement stations marked as bold magenta circles. Only at the eastern boundary does the transect pass through the measurement point. The other transects have the other stations at or near their endpoints.



Figure 3-46. Transect along part of the southern boundary 2004-04-28 (corresponding to JD 119 after 2004-01-01) going westward toward station Si23, but not reaching it. The surface current sets to the west while at about 15 m depth the lower layers are mostly going in the other direction. Even though station Si23 is somewhat to the left of the diagrams the currents measured by the stationary ADCP instrument data (Figures 3-22 and 3-23) are not inconsistent with these vessel-mounted data. The diagrams span close to two nautical miles and give thus an appreciation of the variability within one grid cell of the Baltic CR-model.



Figure 3-47. Transect along part of the southern boundary 2004-07-07 (corresponding to JD 189 in Figures 3-22 and 3-23) going westward. The route is very similar to the one in Figure 3-46 which is reflected by the bottom contours (coarse black line), but the surface current direction is reversed and the feeble current of the bottom layer is flowing southward. The homogeneity of the flow pattern representing one grid cell of the Baltic CR-model is convincingly apparent. Comparison to the measurements with the stationary ADCP deployed at the station Si23 is not easy due to the weak current intensities but at least there are no obvious inconsistencies between these measurements.



Figure 3-48. Transect along part of the northern boundary 2004-10-20 going westward toward station Si21b but not reaching it. The homogeneity of the diagrams that span one grid cell of the Baltic CR-model is fully acceptable even though there is a slight deepening of the surface layer to the east. The date of this transect corresponds to JD 294 in Figures 3-22 and 3-23 and a comparison to these stationary ADCP measurements is again hampered by the weak currents.



Figure 3-49. Transect along part of the northern boundary 2005-04-13 going eastward from station Si21b. This date corresponds to JD 469 in Figures 3-22 and 3-23 representing the very last measurement data. In fact this transect was taken a couple of hours after the stationary ADCP instrument was lifted out of water. In addition, the current magnitude diagram (upper panel) indicates very weak currents. Because of this, the heterogeneity displayed for the horizontal layers, shifting from currents setting northward in the right half of the diagram to currents setting westward in the left half, cannot be interpreted as an indication of current features appearing on a sub-grid cell level.



Figure 3-50. Transect along part of the eastern boundary 2005-04-13 going southward. The approximate position of the station Si22 is indicated by a broken red line. The vessel-mounted ADCP instrument gives current readings down to about 40 m. Beyond this range only scattered data are occasionally given. At the date of this transevct, the current meter at Si22 was at a depth of 49 m. This fact completely dismisses any possibility for making comparisons. The upper velocity magnitude diagram shows an almost ideal homogenous current pattern with weak current down to the 30-m level. From this level and downward a south-going current intensifies across the two nautical mile range.

4 Discussion

4.1 Comparison of currents

As for the parallel study of the Forsmark coastal area /Engqvist and Andrejev 2008/ the argument presented by Andrejev and Sokolov /Andrejev and Sokolov 1989/ still applies to the present study, namely that spectral comparison possibly would be the most adequate way of evaluating modelled current results against measurements. Moreover, if the current direction information is neglected by comparing only the speed of the current, then the overall spectral appearances can be compared irrespective of possible bathymetrical forming and deflection of the flow field. A spectral agreement with regard to the distribution of the variance (Figures 3-11, 3-26 and 3-44 then should be a reflection of a set of forcing (Table 2-1) that is balanced both to its relative magnitude and temporal resolution. If so, the statistical distribution of velocities should also be mainly congruent with regard to the frequency.

In contrast to the earlier performed validation of the Forsmark coastal area, the present current comparison is considerably more favorable. The results in Table 2-3 can be summarized in that at least one of the principal U- or V- components is acceptable, spanning the range from 5% to almost 50% with an average of 30%. The low end of this range is represented by the problematic station Si22 which instrument was inadvertently dislocated to at least two different depths. The high end of the same range consists of the instrument placed in the narrows of Djupesund (Si25). The spectral comparison of measured and simulated data at Si25 shows a close similarity (Figure 3-44) which can be attributed to similarities not only to realistic forcing, but also to the model's capacity to capture the dynamic response of this forcing. In this diagram there is also low-frequency (about 1.5 per day) variance in the measured spectrum that is not matched by the simulated spectrum. The latter, on the other hand has variance on the high-frequency end of the axis that is cut off by the Nyquist limit of the measured one. This provides a plausible explanation of the found aberration between the fluctuations of the salinity and temperature measurements in Figure 3-39. The graphical resolution of this figure may not show this but in fact, the model performs the exchange more frequently and in smaller transactions so that the total exchange over longer time periods is mainly equal to the measured rate. This is substantiated by the curves being closely aligned.

The transects (Figures 3-46 through 3-50), though taken in calm weather conditions, indicate a fairly homogeneous flow field on the scale of the chosen horizontal resolution of the Baltic model. This resolution thus is likely sufficient to resolve the flow structure in this area. In rougher weather conditions – with more elevated winds – local eddies may occur. The discrepancies between measured and simulated current components in Figures 3-7, 3-8, 3-22 and 3-23 can then possibly be explained by formation of eddies that may be simultaneous but separated by distances exceeding the length of a couple of CR-grid cells.

4.2 Temperature evaluation

The temperature dynamics displays a distinct seasonal curve that invariably peaks in summer and has a minimum during winter. This is the basic explanation for why most models are capable of producing temperature data for which the correlations are good. The presently simulated temperature data are no exception, with correlations averaging above 0.9 (Table 2-3). However the correlations decrease with depth. The rather crude formulation of the heat exchange through the air/water interface ignores the radiation portions of heating and cooling /e.g. COHERENS 2004/. Temperatures are routinely measured with thermistor sensors that are mainly unaffected by getting clogged by biological growth of epiphytes and can thus be regarded as an example of a fully reliable metrological device.

4.3 Salinity validation

It seems that the most pertinent validation entity is the salinity, because salt is an almost ideal tracer of water exchange. It lacks state transitions (at least at the salinity levels occurring in normal coastal waters) and is from a chemical point of view basically inert. The good correlations obtained at all stations with an average of explaining more than two thirds of all measured salinity variance thus bears a very favorable testimony to the model's capacity to simulate the bulk of water exchange of the entire Laxemar-Simpevarp coastal area. From other studies of coastal embayments around the Baltic coast /e.g. Engqvist 1996/ and the same experience from other Scandinavian sites of investigation /Stigebrandt 1990, Stigebrandt and Aure 1990/, it is well established that the most effective mode of water exchange is the so-called intermediary exchange that is driven by relative density differences between the inside and the outside of an embayment. Since the salinity is the dominant factor in determining the varying horizontal density gradients, it follows that good salinity correlations mean that the water exchange is adequately modeled.

The malfunction of the salinity sensors for instruments in the photic zone near the surface, in particular during the production season in summer, is a known hazard (Björn Kjerfve pers comm) impeding all salinity measurements based on conductivity measurement as a proxy for salinity. In this study there have been several occasions when this ailment has occurred also while the salinity seems to be decreasing for regular oceanographic reasons. This makes it even more difficult to discriminate between which salinity data should be retained for the statistical analysis and which should be discarded.

As a bonus, the executioner of the field program (SMHI) undertook a series of complementary salinity and temperature measurements so as to produce profiles of these entities with enhanced vertical resolution /Lindow 2005/. This was achieved by casting an assumingly well-calibrated CTD instrument at the stations while the deployed meters were still in operation before lifting and after redeploying the instruments for data retrieval. These comparisons mostly confirmed that the deployed instrument complied within the specified inaccuracies with only a few notable exceptions. One concerns station Si21 2004-06-09 for which there was a 2-unit discrepancy in the psu scale. The probable explanation for this difference is the growth of epiphytes that seemingly had not sufficiently been removed during servicing.

The good salinity correlations found in the present study for the peripheral instruments deployed at the interface between the two 3D-models are in stark contrast to what was found for the parallel study of the Forsmark area and thus begs an explanation. The interior station of the Forsmark study (Fo13) gave comparable results to the interior station of the present study (Si24) with only somewhat lower correlation coefficients.

In the present study the Baltic model data have been indiscriminately used for comparison of the stations located on the boundary between the CR- and the FR-models, while for the Forsmark area the comparison was made to the local model. This cannot provide an explanation for the differing correlation levels since the boundary data from the Baltic model are imposed on local model in such a way that only minor deviations should arise.

Instead, the most plausible explanation must be found in the long-term behavior of the Baltic model. For the Forsmark coastal area the induced residual south-flowing current is occasionally interrupted by wind-induced reverse currents and the fronts of freshwater (from the collective discharge of all rivers in Gulf of Bothnia, in particular the nearby Dalälven) meeting with more saline Baltic Proper water, causing a delicate balance of advection and mixing that the model cannot uphold for extended time periods. This problem does not to the same extent affect the more open Laxemar-Simpevarp coast with a much larger adjacent water body with radically reduced formation of fronts. This hypothesis has been considerably strengthened by a control run with the lately provided Mueller data replacing the previously used Mesan data set. This data set yields for the Forsmark area a noticeably different boundary forcing, which is an indication of how sensitive the local results may be to the large-scale CR-model meteorological forcing.

5 Conclusions

The overall good salinity and temperature (but only comparatively good current speed component) correlations found in this study give reassuring credibility to the combined model effort to simulate the water exchange of the coastal section off the Laxemar-Simpevarp area. This in turn ascertains that the overall wind-moderated and density-driven coastal water exchange is realistically modeled, indicating that both the modeling and the validating approaches are adequately designed.

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