SF_ATBD

M Johnson mjohnson@bmrs.ie

Contents

1 Introduction

1.1 scope and design philosphy

The models presented here aim to meet the requirements of the funder, to predict the 'carrying capcity' of european waters to support shellfish growth, and to be able to make predictions on 3 different species of shellfish. The models need to be able to make predictions at the km scale over the entirety of European waters. As such, the models need to be as simple as possible to keep the uncertainty on the results constrained. This is a significant challenge and two alternative approaches are provided. Firstly, a published, multi-species prognostic dynamic energy balance (DEB) model of shellfish growth (Hawkins et al., 2013) is adapted for these purposes. Secondly a novel steady state model of carrying capacity is derived which takes a single species-specific parameter. Both models are presented in full detail in this ATBD.

2 Prognostic model

The DEB model of Hawkins et al. (2013) is a growth model driven by food availability and energy balance. Growth rates are predicted based on paramerterised growth functions which modulate reference rates by growth conditions e.g. temperature, energy balance.

2.1 Summary

The ShellSim DEB shellfish model developed by Hawkins et al. (2013) was selected as the primary shellfish model for this project as it is the only published shellfish model fully documented in the peer reviewed literature which has been parameterised for mutliple species, including the three target species for this project: The blue mussel *M. Edulis*, king scallop *P. Maximus* and Pacific oyster *C. Gigas*. The model has been re-implemented for this project and, as well as some corrections / fixes to the model as published in order to make the model self-consistent, a very simple population model has been implemented to scale the ShellSim individual model to the farm level. The model is stable and produces reasonable results but our ability to tune and constrain the model accross the whole domain is limited.

2.1.1 Inputs and parameter values

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.1 --
```

Table 1: Environmental forcings to the shellfish model

forcing	description	units
SST	sea surface temperature	°C
CHLA	chlorlophyll concentration	μg/l
PhytoC	Phytoplankton carbon concentraion (optional)	μg/l
POC	Particulate organic carbon (optional)	μg/l
F_{in}	Water current flow rate	m d^{-1}
z_{mix}	vertical mixing length term	m

```
## v tibble  3.1.7     v dplyr   1.0.9
## v tidyr   1.2.0     v stringr 1.4.0
## v readr   2.1.2     v forcats 0.5.1
## v purrr   0.3.4
```

```
## -- Conflicts ---------------------------------------- tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```
## Warning in file(con, "r"): cannot open file '../
## shellfish_model_parameters.json': No such file or directory
```

2.2 Model description

Our implementation of ShellSIM is driven by organic matter availability in seawater and current speed (determining the inputs to the farm). A simple population model reduces the population proportionally when there is insufficient food to support the number of individuals per unit volume. Where we have deviated from (Hawkins et al., 2013), or where the descritption of the model by Hawkins et al. (2013) required clarification we document in full below. Otherwise, for justification of structure or values of hard-coded numerical coefficients the reader is directed back to the source model as described in Hawkins et al. (2013). For the most part we have kept variable names as defined in Hawkins et al. (2013) for traceability.

The state variables of the individual shellfish DEB model are shell energy (SHE) and soft tissue energy (STE).

SHE and STE are related to the dry shell and dry soft tissue weights (DSHW and DSTW respectively) by energy content of shell and tissue, ECS and EST, respectivelty, in J/(dry)mg:

$$\text{DSHW} = \frac{\text{SHE}}{\text{ECS} \cdot 1000} \tag{1}$$

$$\text{DSTW} = \frac{\text{STE}}{\text{EST} \cdot 1000} \tag{2}$$

2.2.1 Ingestion

Chlorophyll-*a* (henceforth Chl*a*) concentration, with or without particulate organic carbon (POC; from which to derive detrital carbon) is used to calculate food availability. Note that ShellSIM can also run with total particular organi matter (POM) instead of POC but given data availability for this project, POC was selected as being preferable. Given the availability of phytoplankton carbon concentration in water (henceforth C_{phyto}) in some CMEMS model outputs we have also implemented the use of POC and C_{phyto} together).

If Chl*a* (in μg/l) is the sole food input to the model then all food intake is treated as preferentially ingested material, SELORG, in mg/l and calculated as

$$\text{SELORG} = \frac{\text{Chl}a \cdot 50}{0.38} \tag{3}$$

Table 2: Shellfish species-specific parameters

parameter	description	units
CR_max	Maximum cleranace rate	l/hr/g DST
CR_grad	Gradient of clearance rate with temperature	
CR_inflec	Temperature of max clearance rate (inflection point of curve)	celcius
a_TEM	species-specific exponent scaling factor for temperature-dependence of maintenance heat loss	
m_NSO	Gradient of relationship between concentration of phytoplankton-derived organic matter (SELORG) and net ingestion rate of SELORG	
c_NSO	Intercept of relationship between concentration of phytoplankton-derived organic matter (SELORG) and net ingestion rate of SELORG i.e. net ingestion rate at zero SELORG	mg/hr/g DST
a_NRO	'a' coefficient of relationship describing net ingestion rate of other organic matter	
b_NRO	'b' exponent of relationship describing net ingestion rate of other organi matter	
ON_min	Minimum consumed O: excreted N (when net energy assimilation is ~zero)	
ON_max	Maximum consumed O: excreted N (when net energy assimilation is max)	
MNEA	Maximum net energy absorbtion	(J/g DST/d)
MTA	Mean tissue allocation between shell and tissue	
WCS	Fractional water content of shell	
WCT	Fractional water content of soft tissue	
SCW	Shell cavity water scaling factor for calculation of wet weight	
a_SHL	'a' coefficient of shell length relationship with dry shell weight	
b_SHL	'b' exponent of shell length relationship with dry shell weight	
SLM	Shell length on maturation	cm
PSTL	Proportion of soft tissue loss on spawning	
TTS	Minimum temperature for spawning	(celcius)
EST	Energy content of dry soft tissue	(J/mg)
ECS	Energy content of dry shell	(J/mg)
h_SF	height of shellfish growth system e.g. ropes / trestles	(m)
stocking_density	stocking density	(/m^3)
specific_mortality	daily fractional mortality	(/d)
protein_DW_fraction	protein content as a fraction of dry weight	

Where POC and Chl$a$ are provided (in μg/l), SELORG and the remaining detrital fraction, REMORG, all in mg/L are calculated separately.

$$\text{SELORG} = \frac{\text{Chl}a \cdot 12}{0.38} \tag{4}$$

$$\text{REMORG} = \frac{2.33 * POC}{1000} - \text{SELORG} \tag{5}$$

Where C_{phyto} is available directly, and where POC is also available, SELORG can alternatively be calculated as

$$\text{SELORG} = \frac{2 \cdot \text{C}_{\text{phyto}}}{1000} \tag{6}$$

Where C_{phyto} is multiplied by 2 to convert from carbon to total mass.

The net ingestion rate of SELORG, NIRSELORG, in mg/hr is then

$$\text{NIRSELORG} = \text{m}_{\text{NSO}} \cdot \text{SELORG} \cdot \text{TEF} \cdot \text{DSTW}^{0.62} \tag{7}$$

Here, m_{NSO} is the (species specific) empirically-derived gradient of the linear fit of observations of ingestion rate with differing SELORG concentrations. DSTW is the dry soft tissue weight in g and TEF is a temperature-based scaling factor derived from the ratio between predicted clearance rates at temperature, T and the predicted clearance rate at 15 Celcius:

$$\text{TEF} = \frac{\text{CR}_{\text{T}}}{\text{CR}_{15}} \tag{8}$$

Hawkins et al. (2013) present different functional forms of the clearance rate-temperature relationship for different species. Here we standardize the clearance rate-temperature for any species to the form:

$$\text{CR} = \text{CR}_{\text{max}} - \text{CR}_{\text{grad}} \cdot (\text{T} - \text{CR}_{\text{inflec}})^2 \tag{9}$$

Where CR_{max} is the maximum clearance rate, $\text{CR}_{\text{inflec}}$ is the temperature at which maximum clearance rate is observed. CR_{grad} is the 'gradient' term used to fit to the observed data.

The ingestion rate of REMORG, NIRREMORG, in mg/hr, is given by

$$\text{NIRREMORG} = \text{a}_{\text{NRO}} \cdot \left(1 - e^{\text{b}_{\text{NRO}} \cdot \text{REMORG}}\right) \cdot \text{TEF} \cdot \text{DSTW}^{0.62} \tag{10}$$

where a_{NRO} and b_{NRO} are species specific parameters. Net energy assimilation NEA in J/d is calculated from NIRREMORG and NIRSELORG as follows:

$$\text{NEA} = 24 \cdot \epsilon_{\text{assim}} \left(\text{NIRSELORG} \cdot \text{ESELORG} + \text{NIRREMORG} \cdot \text{EREM} \cdot \Phi\right) \tag{11}$$

Here, 24 converts from per hour to per day, ϵ_{assim} is the assimilation efficiency (0.82 in Hawkins et al. (2013)); ESELORG is the energy content of SELORG and EREM the energy content of REMORG, assigned default values of 23.5 and 20.48 J/mg respectively in Hawkins et al. (2013). Φ is the fraction of REMORG that is bioavailable, fixed at 0.15 in the model description of Hawkins et al. (2013).

2.2.2 Maintenance and net energy balance

Maintenance heat loss, MHL in J/day is

$$\mathrm{MHL} = 96.12 \cdot \mathrm{TEF} \cdot \mathrm{DSTW}^{0.72} \tag{12}$$

where 96.12 is 4.005 J/h/g from Hawkins et al. (2013) multiplied by 24 hours.

Total heat loss THL also in J/day is then

$$\mathrm{THL} = \mathrm{MHL} + 0.23\mathrm{NEA} \tag{13}$$

In Hawkins et al. (2013) it is stated that "... according to Hawkins et al. (2002) ... the fractional energy cost of feeding and digestion [is] based on measures of ... 0.23 J/g/hr". This statement is not self-consistent as a fractional energy cost should be unitless and indeed on referring back to Hawkins et al. (2002) we find 0.23 defined as the "Heat loss per unit energy absorption above maintenance" and with stated units of J/J (i.e. unitless). We conclude Hawkins et al. (2002) must be correct and the 0.23 is a unitless 'energy cost' as they define it.

Hawkins et al. (2013) model excretory energy losses by relating them to the O:N ratio of respiration (with lower O:N when the shellfish have less food).

O:N ratio is explained by Widdows (1978) as:

> "... the oxygen:nitrogen ratio (O:N) [...] is the ratio of oxygen consumed to nitrogen excreted, in atomic equivalents; it provides an indication of the balance in the animal's tissues between the rates of catabolism of protein, carbohydrate and lipid substrates (Corner & Cowey, 1968; Bayne, 1973 a, 1975; Bayne et al. 1976). A low value for O:N indicates that mainly protein is being utilized; whereas a high value indicates catabolism of carbohydrate and/or fat. The theoretical minimum for the O:N ratio is approximately 7 (Mayzaud,1973) signifying catabolism based entirely upon protein."

O:N is calculated assuming a linear relationship with NEA where O:N varies from minimum to maximum species specific observed values as NEA varies from 0 to species specific maximum observed value MNEA.

As stated by Hawkins et al. (2013):

$$\mathrm{O:N} = 10 + (((200 - 10) \div \mathrm{MNEA}) \times \mathrm{NEA}) \tag{14}$$

Parameterised for use here with multiple species (note that scallops have different max O:N):

$$\mathrm{O:N} = \mathrm{O:N}_{min} + \frac{\mathrm{O:N}_{max} - \mathrm{O:N}_{min}}{\mathrm{MNEA}} \cdot \mathrm{NEA} \tag{15}$$

Excretory loss (EL) in μg NH_4-N/day (stated incorrectly by Hawkins et al. (2013) as μg NH_4/day) is then calculated as a function of the total heat loss converted to oxygen and then converted on to NH4 via the O:N ratio. Hawkins et al. (2013) describe this as:

$$\mathrm{EL} = (((THL \div 14.06) \div 16) \div \mathrm{O:N}) \times 14 \times 1000 \tag{16}$$

Here $\frac{\mathrm{THL}}{14.06}$ gives the oxygen equivalents of the total heat loss. Further dividing by 16 (should be 32... see below) converts to (milli)molar units, then dividing by O : N gives the NH4 equivalents in (milli)molar units, multiply by 14 to convert to mg NH4-N, by 1000 for μg. Note there is a spurious $\times 24$ in the text description of this equation in Hawkins et al. (2013).

Teasing this all apart... Hawkins et al. (2013) state that "1 mg O_2 = 14.06 J". What is meant by this is that the energy involved in the use of 1mg of oxygen in respiration is 14.06J. They refer to Gnaiger (1983) for this value. In this work, in Table 4 of Gnaiger (1983), the heat loss associated with 1 μmol O_2 consumption per hour is given as 0.45 J/hr. 1 μmol O_2 is equivalent to ($\times\frac{32}{1000}$) = 0.032 mg. Therefore, energy per mg is 0.45/0.032 = 14.06 J/mg. Hawkins et al. (2013) incorrectly use rmm of oxygen not O_2 (i.e. 16 rather than 32 to convert back to a molar quantity in the calculation of EL).

We correct this error and re-state the EL equation as follows

$$\mathrm{EL} = \frac{\mathrm{THL}}{0.450 \cdot \mathrm{O:N}} \cdot 14 \tag{17}$$

Where 0.450 converts 1J of energy loss to oxygen equivalents in μmol O_2 directly as described in Gnaiger (1983), which results in a simpler conversion via O : N and the rmm of nitrogen to give μg NH_4-N.

EL is used with a conversion factor from ammonium back to energy and subtracted, along with THL, from NEA to give the net energy balance NEB in Joules (per day):

$$\mathrm{NEB} = \mathrm{NEA} - \mathrm{THL} - (\mathrm{EL} * 0.0248) \tag{18}$$

The conversion from NH_4 to energy (0.0248 J per μg NH_4-N) compares well to the heat of combustion of NH_4 quoted in Pilgrim (1954) (~0.021 when converted to the same units), whose paper is also about energy loss via excretion of reduced N compounds.

2.2.3 growth

Shell and soft tissue growth, and spawning are controlled in the model by the condition variable, COND.

$$\mathrm{COND} = \frac{\mathrm{STE}}{\mathrm{STE} + \mathrm{SHE}} \tag{19}$$

Shell growth (SHG) occurs when COND surpasses a species-specific threshold value mean tissue allocation (MTA) and when there is net energy increase.

$$\mathrm{SHG} = \begin{cases} \mathrm{NEB} \cdot (1 - \mathrm{MTA}), & \mathrm{COND} \geq \mathrm{MTA\&NEB} > 0 \\ 0, & otherwise \end{cases} \tag{20}$$

Soft tissue growth (STG) only occurs when NEB > 0 and is calculated as

$$\mathrm{STG} = \begin{cases} \mathrm{NEB} \cdot \mathrm{MTA}, & \mathrm{COND} \geq \mathrm{MTA\&NEB} > 0 \\ \mathrm{NEB}, & \mathrm{COND} < \mathrm{MTA\&NEB} > 0 \\ 0, & \mathrm{NEB} \leq 0 \end{cases} \tag{21}$$

The rate of change of the state variables shell energy, SHE and soft tissue energy STE are then equal to SHG and STG, respectively

$$\frac{d\mathrm{SHE}}{d\mathrm{t}} = \mathrm{SHG} \tag{22}$$

$$\frac{d\mathrm{STE}}{d\mathrm{t}} = \mathrm{STG} \tag{23}$$

2.2.4 Spawning

When the conditions are right, bivalves will spawn, loosing soft tissue weight. Spawning occurs in the model when the temperature surpasses a minimum value, TTS, when the organisms have reached or exceeded their mature shell length, SLM; and when COND is greater than 0.95 of MTA. Furthermore, no more than 2 spawning events are permitted per rolling year-long period.

On spawning, a percentage of soft tissue weight is lost (PSTL). TTS, SLM and PSTL are all species specific parameters.

2.2.5 Population model

In order to scale up from the individual-based DEB model outlined above, to the farm scale, we implement here a simple population model which tracks the number of invidiuals per cubic metre of water. On initialisation of the model, the population is set to the value of the stocking density per m^3. Subsequently whenever NEB is negative, population is lost in order to maintain energy requirements in the remaining organisms:

$$\frac{d\mathrm{POP}}{d\mathrm{t}} = \begin{cases} \mathrm{POP} \cdot \frac{\mathrm{NEB}}{\mathrm{STE}}, & \mathrm{NEB} < 0 \\ 0, & \mathrm{NEB} \geq 0 \end{cases} \tag{24}$$

2.3 Derived variables

Fresh weight, Drained wet weight and Shell length are calculated according to Hawkins et al. (2013).

2.3.1 Protein content

Protein content as fraction of dry soft tissue weight.

Mussel (M. edulis): 0.2-0.3 (assume average 0.25) (Pleissner et al., 2012) Oyster (C. Gigas): 0.5-0.57 (commercial population 0.53) (Zhu et al., 2018)

Scallop P. Maximus Cortés et al. (2021) 19% by cooked weight assume no loss of moisture on cooking so assume 19% protein in drained wet tissue weight. DWW:DSTW = 1.914 so protein content = 0.19 * 1.914 = 0.26796

2.3.2 Energy content

Energy content per individual is directly modelled by the DEB model. Energy content is therefore acessible in the model output - scaled to total farm output and per m2 as per other output variables.

2.4 Reference runs

Need documenting

```
source("run_SF.R")
```

```
## Warning in file(con, "r"): cannot open file '../
## shellfish_model_parameters.json': No such file or directory
```

```
HL<-reference_run(hclf,c(PHYC_data=FALSE))
LL<-reference_run(lclf,c(PHYC_data=FALSE))
LH<-reference_run(lchf,c(PHYC_data=FALSE))
HH<-reference_run(hchf,c(PHYC_data=FALSE))

  HL$run<-'hclf'
  LL$run<-'lclf'
  LH$run<-'lchf'
  HH$run<-'hchf'
```

```
  refruns<-rbind(HL,LL,LH,HH)

a<- ggplot(refruns) +
  aes(x = time, y = CHL_farm, colour = run) +
  geom_point(shape = "circle", size = 0.7) +
  scale_color_hue(direction = 1) + ylab("CHL / ug.l^-1")+
  theme_minimal()
 b<-  ggplot(refruns) +
  aes(x = time, y = POC_farm, colour = run) +
  geom_point(shape = "circle", size = 0.7) +
  scale_color_hue(direction = 1) + ylab("POC / ug.l^-1")+
  theme_minimal()
 c<-  ggplot(refruns) +
  aes(x = time, y = SHL, colour = run) +
  geom_point(shape = "circle", size = 0.7) +
  scale_color_hue(direction = 1) + ylab("Shell length / cm")+
  theme_minimal()
  d<-   ggplot(refruns) +
  aes(x = time, y = NH4_production, colour = run) +
  geom_point(shape = "circle", size = 0.7) +
  scale_color_hue(direction = 1) + ylab("NH4 yield / g.d^-1 ")+
  theme_minimal()

 e<-  ggplot(refruns) +
  aes(x = time, y = DSTW_PUA, colour = run) +
  geom_point(shape = "circle", size = 0.7) +
  scale_color_hue(direction = 1) + ylab("Dry soft tissue / kg.m^-2")+
  theme_minimal()
  f<-   ggplot(refruns) +
  aes(x = time, y = FW_PUA, colour = run) +
  geom_point(shape = "circle", size = 0.7) +
  scale_color_hue(direction = 1) + ylab("Fresh weight / kg.m^-2")+
  theme_minimal()

 (a|b)/(c|d)/(e|f)
```

```
source("run_SF.R")
```

```
## Warning in file(con, "r"): cannot open file '../
## shellfish_model_parameters.json': No such file or directory
```

```
HL<-reference_run(hclf,c(PHYC_data=FALSE),species='Cgig')
LL<-reference_run(lclf,c(PHYC_data=FALSE),species='Cgig')
LH<-reference_run(lchf,c(PHYC_data=FALSE),species='Cgig')
HH<-reference_run(hchf,c(PHYC_data=FALSE),species='Cgig')

  HL$run<-'hclf'
  LL$run<-'lclf'
  LH$run<-'lchf'
  HH$run<-'hchf'

  refruns<-rbind(HL,LL,LH,HH)

a<- ggplot(refruns) +
```

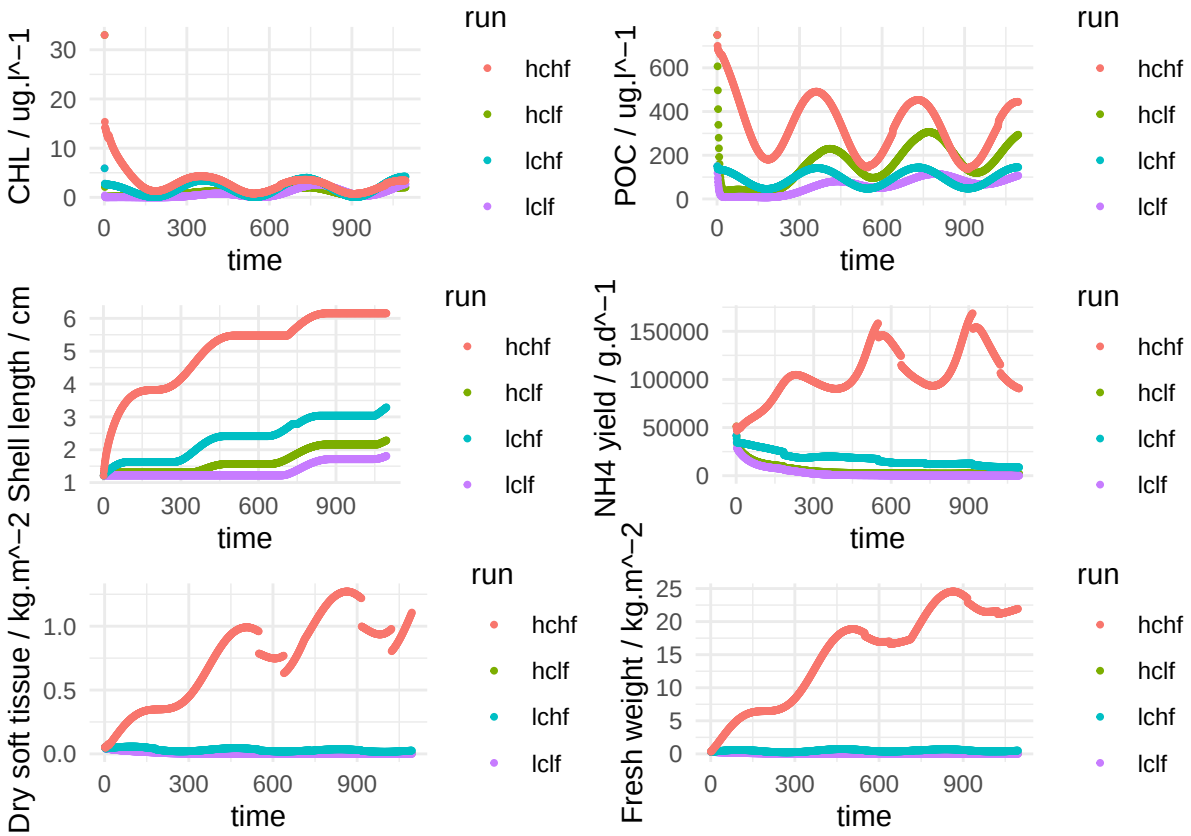

Figure 1: (#fig:refrun_Medulis)Reference runs of the model for M edulis, showing a) Chlorophyll concentration within the farm (ug/l) b) POC concentration in the farm (ug/l), c) Individual shell length (cm) ,d) daily NH4 production accross the farm (1km*1km), e) soft tissue biomass (dry weight) per unit area (kg/mˆ2) and f) Fresh weight per unit area (kg/mˆ2)

```
 aes(x = time, y = CHL_farm, colour = run) +
 geom_point(shape = "circle", size = 0.7) +
 scale_color_hue(direction = 1) + ylab("CHL / ug.l^-1")+
 theme_minimal()
b<-  ggplot(refruns) +
 aes(x = time, y = POC_farm, colour = run) +
 geom_point(shape = "circle", size = 0.7) +
 scale_color_hue(direction = 1) + ylab("POC / ug.l^-1")+
 theme_minimal()
c<-  ggplot(refruns) +
 aes(x = time, y = SHL, colour = run) +
 geom_point(shape = "circle", size = 0.7) +
 scale_color_hue(direction = 1) + ylab("Shell length / cm")+
 theme_minimal()
 d<-   ggplot(refruns) +
 aes(x = time, y = NH4_production, colour = run) +
 geom_point(shape = "circle", size = 0.7) +
 scale_color_hue(direction = 1) + ylab("NH4 yield / g.d^-1 ")+
 theme_minimal()

e<-  ggplot(refruns) +
 aes(x = time, y = DSTW_PUA, colour = run) +
 geom_point(shape = "circle", size = 0.7) +
 scale_color_hue(direction = 1) + ylab("Dry soft tissue / kg.m^-2")+
 theme_minimal()
 f<-   ggplot(refruns) +
 aes(x = time, y = FW_PUA, colour = run) +
 geom_point(shape = "circle", size = 0.7) +
 scale_color_hue(direction = 1) + ylab("Fresh weight / kg.m^-2")+
 theme_minimal()

(a|b)/(c|d)/(e|f)
```


Cortés, A., González-García, S., Franco-Uría, A., Moreira, M. T., & Feijoo, G. (2021). Evaluation of the environmental sustainability of the inshore great scallop (pecten maximus) fishery in galicia. *Journal of Industrial Ecology*. https://doi.org/10.1111/jiec.13153

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Widdows, J. (1978). Physiological indices of stress in mytilus edulis. *Journal of the Marine Biological Association of the U.K*, 125–142.

Zhu, Y., Qi, L. I., Hong, Y. U., & Lingfeng, K. (2018). Biochemical composition and nutritional value of different shell color strains of pacific oyster crassostrea gigas. *J. Ocean Univ. China (Oceanic and Coastal*

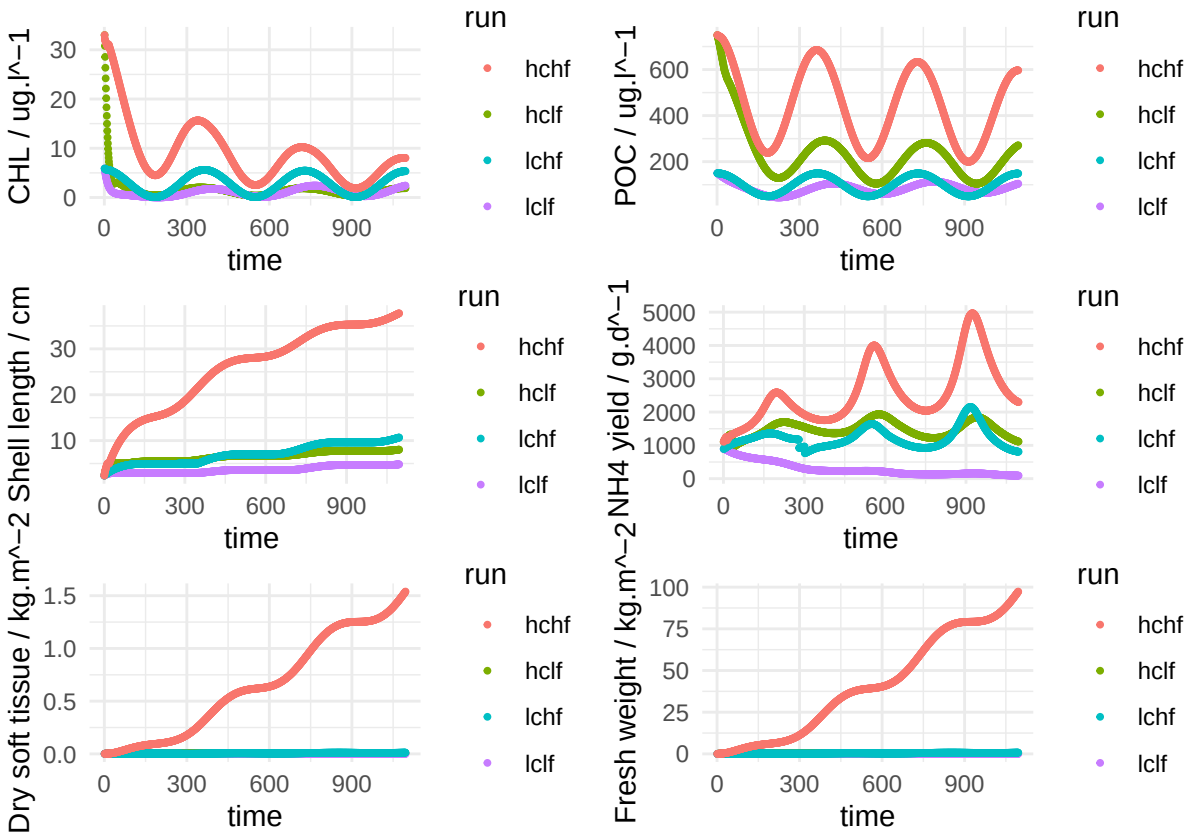

Figure 2: (#fig:refrun_Cgigas)Reference runs of the model for C gigas, showing a) Chlorophyll concentration within the farm (ug/l) b) POC concentration in the farm (ug/l), c) Individual shell length (cm) ,d) daily NH4 production accross the farm (1km*1km), e) soft tissue biomass (dry weight) per unit area (kg/mˆ2) and f) Fresh weight per unit area (kg/mˆ2)

Sea Research, *17*, 897–904. https://doi.org/10.1007/s11802-018-3550-6