A User Guide to the PROCESS Fusion Reactor Systems Code

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Contents

List of Figures

List of Tables

Chapter 1

Introduction

1.1 Rationale

During the course of studies into a proposed fusion power plant, there may be times when questions of the following type arise:

> Are the machine's physics and engineering parameters consistent with one another?
>
> Which machine of a given size and shape produces the cheapest electricity?
>
> What is the effect of a more optimistic limit on the maximum plasma density on the amount of auxiliary power required?

Questions such as these are extremely difficult to answer, since the large number of parameters involved are highly dependent on one another. Fortunately, computer programs have been written to address these issues, and `PROCESS` is one of them.

Suppose that an outline power plant design calls for a machine with a given size and shape, which will produce a certain net electric power. There may be a vast number of different conceptual machines that satisfy the problem as stated so far, and `PROCESS` can be used in "non-optimisation" mode to find one of these whose physics and engineering parameters are self-consistent. However, the machine found by `PROCESS` in this manner may not be possible to build in practice — the coils may be overstressed, for instance, or the plasma pressure may exceed the maximum possible value. `PROCESS` contains a large number of constraints to prevent the code from finding a machine with such problems, and running the code in so-called "optimisation" mode forces these constraints to be met. The number of possible conceptual machines is thus considerably reduced, and optimisation of the parameters with respect to (say) the cost of electricity will reduce this number to a minimum (possibly one).

Formally then, `PROCESS` is a systems code that calculates in a self-consistent manner the parameters of a fusion power plant with a specified performance, ensuring that its operating limits are not violated, and with the option to optimise a given function of these parameters.

1.2 History

`PROCESS` is derived from several earlier systems codes, but is largely based on the TETRA (Tokamak Engineering Test Reactor Analysis) code [1] and its descendant STORAC (Spherical TOrus Reactor Analysis Code) [2], which includes routines relevant to the spherical tokamak class of machines. These codes, and much of the original version of `PROCESS` itself, were written by personnel at Oak Ridge

National Laboratory in Tennessee, USA, with contributions from a number of other laboratories in the USA. In addition, many of the mathematical routines have been taken from a number of different well-established source libraries.

A great deal of effort was expended at Culham on the code's arrival from ORNL in the early 1990s to upgrade and extend the code, including the addition of machines based on the stellerator, reversed field pinch and inertial confinement concepts.

`PROCESS` is being developed actively. This User Guide is updated in parallel with the code itself to ensure that the documentation remains consistent with the latest version of the code. It is to be hoped that it will be of assistance not only to users of `PROCESS`, but to anyone using `PROCESS` outputs or models based on them.

1.3 Sources of information

The output file OUT.DAT contains details of all the constraints and iteration variables selected, the input and output parameters, and which models have been chosen. It is essential to study the full output before using the results in any way.

Details of the physics, engineering and cost models are being published:

[19]: M. Kovari et al., PROCESS: a systems code for fusion power plants - Part 1: Physics

[20]: M. Kovari et al., PROCESS: a systems code for fusion power plants - Part 2: Engineering, in preparation

[21]: M. Kovari et al., The cost of a fusion power plant: extrapolation from ITER, in preparation

To view sample input and output files and a description of the variables, or to report bugs, request improvements, propose new models, or contact the `PROCESS` developers, please visit

ccfe.ac.uk/powerplants.aspx.

Chapter 2

Program Overview — The Fundamental Concepts

Fusion power plants are complex systems consisting of many non-linear interactions. One method that can be used to model this kind of system is to iterate a number of free parameters (the so-called *iteration variables* — see Section 2.4) in a controlled way so as to find a self-consistent set of device parameters that satisfy all of the system's *constraint equations* — see Section 2.5. `PROCESS` is organised in a standard equation solver format to enable this task to be performed efficiently. The physics and engineering routines together serve as a *function evaluator*, providing the information used in the solution of the constraints. The numerical modules present in `PROCESS` perform the iteration required, and also incorporate the option to maximise or minimise a given *figure of merit* – see Section 2.6.

2.1 Equation Solvers

`PROCESS` contains a constrained non-linear optimiser, and a constrained non-linear equation solver, which reflect the two modes of operation available. Each of these has its own uses, as is now discussed.

2.1.1 Non-optimisation mode

The first of the two equation solvers present in `PROCESS` is the non-optimisation package HYBRD [3, 4]. Formally, HYBRD finds a zero of a system of N non-linear functions in N variables. This means simply that N variables (power plant parameters) are iterated by `PROCESS` in such a way as to solve a set of N equations (physics or engineering laws), i.e. a set of self-consistent power plant parameters is found. This is useful for performing benchmark comparisons, when the device size is kept fixed, and one only wishes to find calculated stresses, beta values, fusion powers, etc. A flow diagram of `PROCESS` in non-optimisation mode is shown in Figure 2.1.

2.1.2 Optimisation mode

Sometimes one wants to find an optimal machine that is both consistent with the physics and engineering constraints but also minimises or maximises a certain *figure of merit*. This requires running `PROCESS` in optimisation mode. For these applications `PROCESS` uses the routine `VMCON` [5] based on a variable metric method for constrained optimisation by Powell [6]. It finds a stationary point of an objective function/figure of merit consistent with a set of equality and inequality constraints

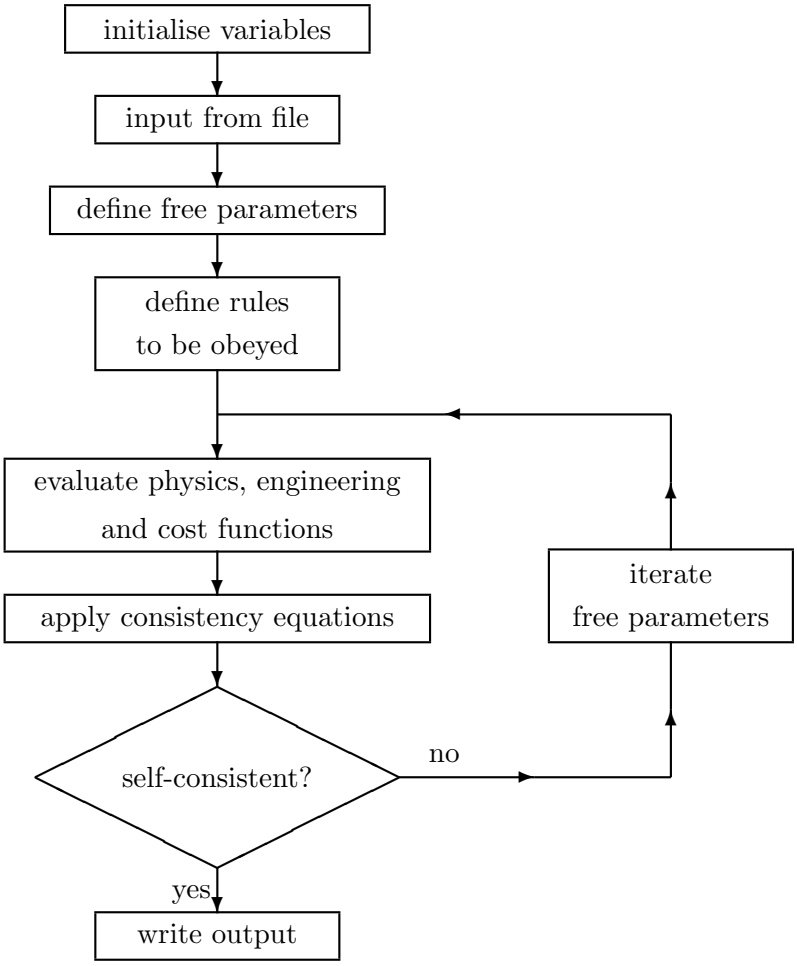


Figure 2.1: *Flow diagram of* `PROCESS` *in non-optimisation mode.*

(see Section A.1). It is designed to solve the necessary but not sufficient conditions of a constrained optimum, hence, the solution does not have to be a global optimum (see Section A.2).

The detailed algorithm is explained in Appendix A and is based on the Lagrange method (see Section A.2) that combines both the objective function and the constraints using Lagrange multipliers. It applies a sequential quadratic programming approach (Section A.3) in which a series of subproblems is solved that constitute a local quadratic expansion of the Lagrangian (Section A.5). The solution of the quadratic subproblem is the direction of a line search along which a one dimensional optimisation is performed (Section A.6). This line search was introduced by Powell to assure convergence from bad starting parameters. Within `PROCESS` we have modified the line search of the original `VMCON` routine to (try to) assure convergence, even for slightly inconsistent input functions.

The algorithm uses a quasi-Newtonian approach which only requires continuous first derivatives of these functions. While the first derivatives are evaluated using a finite difference approximation, the second derivatives are estimated using a variant of the Broyden-Fletcher-Goldfarb-Shanno update (see Section A.7).

The convergence criterion of the solver as well as the detailed interpretation of the various error codes are explained in Section A.4. A flow diagram of `PROCESS` in optimisation mode is shown in Figure 2.2.

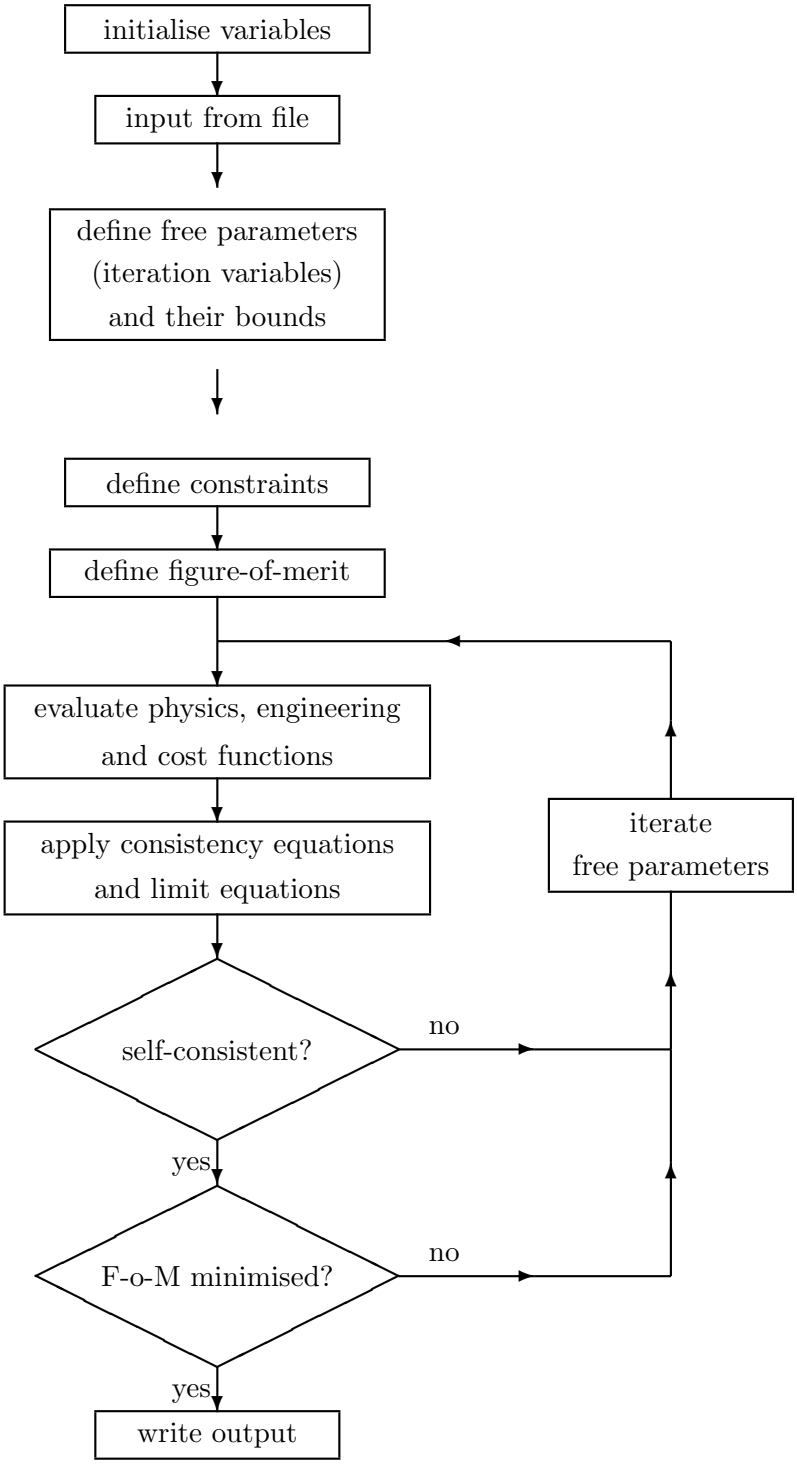


Figure 2.2: *Conceptual flow diagram of* `PROCESS` *in optimisation mode. Please note that this is a simplistic interpretation of the actual sequence of operations, to outline the difference between non-optimisation and optimisation modes. For a more detailed (and correct!)* `VMCON` *flow diagram, please see Figure A.2.*

2.1.3 Scans

It is often useful to be able to scan through a range of values of a given parameter to see what effect this has on the machine as a whole. Sensitivity studies of this kind can be achieved very easily using `PROCESS`. Scans are carried out in optimisation mode, whereby the code initially performs a run using the parameters specified in the input file, and then a series of runs using the parameters produced at the end of the previous iteration. The value of the quantity being scanned is specified at every stage — see Section 2.7. This method ensures that a smooth variation in the machine parameters is achieved. A tool to carry out scans in any number of parameters is under development.

2.2 The Variable Descriptor File

The variable descriptor file `vardes.html` is an invaluable resource for the user of `PROCESS`. It acts as a dictionary / reference manual for the code's variables, and contains the following information about each:

- name
- dimensions (of arrays)
- default value(s)
- description, including physical units if relevant
- for switches/flags, the meanings of all allowed values
- iteration variable number, if relevant
- corresponding constraint equation, if relevant

In addition, global code parameters are labelled `FIX`. These can only be changed by editing the relevant source file, but this should not be carried out unless it is absolutely necessary.

All the variables that are shown with a default value are available to be changed by the user using the input file (Section 4.4), except for those which are labelled `FIX`. Variables not shown with a default value are calculated by the code from a combination of other parameters, and so it would be meaningless to initialise them. Obviously, these variables cannot be changed using the input file.

2.3 Input Parameters

Input parameters make up a large proportion of the variables listed in the variable descriptor file. They comprise all those variables that, once set in the input file (or set to a default value), do not change throughout a `PROCESS` run. For example, the variable `fdeut` is input, and cannot change during a run, appearing in vardes.html as follows: `fdeut /0.5/ :  deuterium fuel fraction`.

2.4 Iteration Variables

Variables that are adjusted by `PROCESS` in order to satisfy the constraints and optimise the figure of merit are referred to as iteration variables. Successive calls are made to the physics and engineering

routines, with slightly different values for the iteration variables on each call, and the equation solver determines the effect on the output due to these small changes to the input (see Figures 2.1 and 2.2). Tables 2.1 and 2.2 list the iteration variables available in `PROCESS`. Any one or more of these variables may be selected.

Clearly, the equation solvers need at least as many variables to iterate as there are equations to solve, i.e. `nvar` $\geq$ `neqns`. If the run is a non-optimising case, then `neqns` variables are iterated — the values of the remaining `(nvar-neqns)` variables are left alone. If the run is an optimising case, then all the active iteration variables are adjusted so as to find the minimum (or maximum) value of a parameter (the *figure of merit*) in the `nvar`-dimensional space of the problem.

In optimisation mode, all the iteration variables are constrained to lie between lower and upper bounds. For instance, the plasma electron density is, by default, confined to lie between the values 10^{19} m^{-3} and 10^{21} m^{-3}. Of course, it can also be constrained to lie below the *calculated* density limit, if constraint equation 5 is activated and the f-value `fdene` (iteration variable no. 9) is bounded by the values 0 and 1.

It is important to remember that iteration variables *must never be initialised to zero.* The code will not be able to adjust the variable's value if this is done, and it will stop with an error message.

For example, the major radius is available as an iteration variable, and appears in the variable description file as `rmajor /8.14/ : plasma major radius (m) (iteration variable 3)`. If it is selected as an iteration variable, it will be adjusted by the code. The value input by the user (or the default, if no value is specified), will be used as the starting value.

ixc no.	variable name	description	icc eqn	lower bound	upper bound
1	aspect	plasma aspect ratio		1.100D0	10.00D0
2	bt	toroidal field on axis		0.010D0	100.0D0
3	rmajor	plasma major radius		0.100D0	10.00D0
4	te	electron temperature		5.000D0	500.0D0
5	beta	plasma beta		0.001D0	1.000D0
6	dene	electron density		1.00D19	1.00D21
7	rnbeam	hot beam density / electron density		1.00D-6	1.000D0
8	fbeta	f-value for $\epsilon.\beta_p$ limit equation	6	0.001D0	1.000D0
9	fdene	f-value for density limit equation	5	0.001D0	1.000D0
10	hfact	confinement time H-factor		0.100D0	3.000D0
11	pheat	heating power not used for current drive		0.001D0	1.000D3
12	oacdcp	overall current density in TF coil inboard leg		1.000D5	1.500D8
13	tfcth	TF coil inboard leg thickness		1.000D0	5.000D0
14	fwalld	f-value for wall load limit equation	8	0.001D0	1.000D0
15	fvs	f-value for volt second limit equation	12	0.001D0	1.000D0
16	ohcth	central solenoid thickness		0.001D0	1.000D2
17	tdwell	dwell time		0.100D0	1.000D8
18	q	edge safety factor		2.000D0	100.0D0
19	enbeam	neutral beam energy		1.000D0	1.000D6
20	tcpav	average (resistive) TF coil temperature		40.00D0	1.000D3
21	ftburn	f-value for burn time limit equation	13	0.001D0	1.000D0
22	tbrnmn	minimum burn time		0.001D0	1.000D6
23	fcoolcp	coolant fraction of resistive TF coil		0.100D0	0.500D0
24	cdtfleg	TF coil leg overall current density		1.000D4	1.000D8
25	fpnetel	f-value for net electric power limit equation	16	0.001D0	1.000D0
26	ffuspow	f-value for fusion power limit equation	9	0.001D0	1.000D0
27	fhldiv	f-value for divertor heat load limit equation	18	0.001D0	1.000D0
28	fradpwr	f-value for radiation power limit equation	17	0.001D0	0.990D0
29	bore	machine bore		0.100D0	10.00D0
30	fmva	f-value for MVA limit equation	19	0.010D0	1.000D0
31	gapomin	minimum gap between outboard vacuum vessel and TF coil		0.001D0	10.00D0
32	frminor	f-value for minor radius limit equation	21	0.001D0	1.000D0
33	fportsz	f-value for beam tangency radius limit equation	20	0.001D0	1.000D0
34	fdivcol	f-value for divertor collisionality limit equation	22	0.001D0	1.000D0
35	fpeakb	f-value for peak toroidal field limit equation	25	0.001D0	1.000D0
36	fbetatry	f-value for beta limit equation	24	0.001D0	1.000D0
37	coheof	central solenoid current density at end of flat-top		1.000D5	1.000D8
38	fjohc	f-value for central solenoid current at EOF limit equation	26	0.010D0	1.000D0
39	fjohc0	f-value for central solenoid current at BOP limit equation	27	0.001D0	1.000D0
40	fgamcd	f-value for current drive gamma limit equation	37	0.001D0	1.000D0
41	fcohbop	central solenoid current density ratio BOP/EOF		0.001D0	1.000D0
42	gapoh	gap between central solenoid and TF coil		0.001D0	10.00D0
43	cfe0	seeded high-Z impurity fraction		1.00D-6	3.00D-3
44	fvsbrnni	fraction of plasma current produced by non-inductive means		0.001D0	1.000D0
45	fqval	f-value for fusion gain limit equation	28	0.001D0	1.000D0
46	fpinj	f-value for injection power limit equation	30	0.001D0	1.000D0
47	feffcd	current drive efficiency multiplier		0.001D0	1.000D0
48	fstrcase	f-value for TF coil case stress limit equation	31	0.001D0	1.000D0
49	fstrcond	f-value for TF coil conduit stress limit equation	32	0.001D0	1.000D0
50	fiooic	f-value for TF coil operational current limit equation	33	0.001D0	1.000D0
51	fvdump	f-value for TF coil dump voltage limit equation	34	0.001D0	1.000D0
52	vdalw	allowable TF coil dump voltage		0.001D0	1.000D6
53	fjprot	f-value for TF coil current protection limit equation	35	0.001D0	1.000D0
54	ftmargtf	f-value for TF coil temperature margin limit equation	36	0.001D0	1.000D0
55		(OBSOLETE)		-	-

Table 2.1: *Iteration variables 1 to 55 present in* PROCESS*. The f-values correspond to the given constraint equations (see Table 2.3). The other iteration variables are shown in Table 2.2.*

ixc no.	variable name	description	icc eqn	lower bound	upper bound
56	tdmptf	dump time for TF coil		10.00D0	1.000D6
57	thkcas	TF coil external case thickness		0.050D0	1.000D0
58	thwcndut	TF coil conduit case thickness		0.001D0	1.000D0
59	fcutfsu	copper fraction of cable conductor		0.001D0	1.000D0
60	cpttf	current per turn in the TF coils		0.001D0	4.000D4
61	gapds	gap between vacuum vessel and inboard TF coil		0.001D0	10.00D0
62	fdtmp	f-value for 1st wall coolant temperature rise limit equation	38	0.001D0	1.000D0
63	ftpeak	f-value for 1st wall peak temperature limit equation	39	0.001D0	1.000D0
64	fauxmn	f-value for minimum auxiliary power limit equation	40	0.001D0	1.000D0
65	tohs	central solenoid current ramp-up time		0.100D0	1.000D3
66	ftohs	f-value for central solenoid current ramp-up time limit equation	41	0.001D0	1.000D0
67	ftcycl	f-value for minimum cycle time limit equation	42	0.001D0	1.000D0
68	fptemp	f-value for maximum centrepost temperature limit equation	44	0.001D0	1.000D0
69	rcool	average radius of centrepost coolant channel		0.001D0	0.010D0
70	vcool	maximum centrepost coolant flow speed at midplane		1.000D0	1.000D2
71	fq	f-value for minimum edge safety factor limit equation	45	0.001D0	1.000D0
72	fipir	f-value for maximum I_p/I_{rod} limit equation	46	0.001D0	1.000D0
73	scrapli	inboard gap between plasma and first wall		0.001D0	10.00D0
74	scraplo	outboard gap between plasma and first wall		0.001D0	10.00D0
75	tfootfi	ratio of TF coil outboard/inboard leg thickness		0.200D0	5.000D0
76	frfptf	f-value for TF coil toroidal thickness limit equation	47	0.001D0	1.000D0
77	tftort	TF coil toroidal thickness (use for RFPs only)		0.050D0	4.000D0
78	rfpth	RFP pinch parameter, Θ		0.010D0	1.800D0
79	fbetap	f-value for poloidal beta limit equation	48	0.001D0	1.000D0
80	frfpf	f-value for RFP reversal parameter limit equation	49	0.001D0	1.000D0
81	edrive	IFE driver energy		1.000D5	5.000D7
82	drveff	IFE driver wall plug to target efficiency		0.010D0	1.000D0
83	tgain	IFE target gain		1.000D0	500.0D0
84	chrad	radius of IFE chamber		0.100D0	20.00D0
85	pdrive	IFE driver power reaching target		1.000D6	2.000D8
86	frrmax	f-value for maximum IFE repetition rate equation	50	0.001D0	1.000D0
87	helecmw	electrical power required for hydrogen production		1.000D0	4.000D3
88	hthermmw	thermal power required for hydrogen production		1.000D0	4.000D3
89	ftbr	f-value for tritium breeding ratio limit equation	52	0.001D0	1.000D0
90	blbuith	inboard blanket breeding unit thickness		0.001D0	2.000D0
91	blbuoth	outboard blanket breeding unit thickness		0.001D0	2.000D0
92	fflutf	f-value for fast neutron fluence on TF coil equation	53	0.001D0	1.000D0
93	shldith	inboard shield thickness		0.001D0	10.00D0
94	shldoth	outboard shield thickness		0.001D0	10.00D0
95	fptfnuc	f-value for TF coil nuclear heating limit equation	54	0.001D0	1.000D0
96	fvvhe	f-value for vessel He concentration limit equation	55	0.001D0	1.000D0
97	fpsepr	f-value for $P_{\text{separatrix}}/R_{\text{major}}$ limit equation	56	0.001D0	1.000D0
98	li6enrich	lithium-6 enrichment percentage (blktmodel=1)		7.400D0	100.0D0
99		(OBSOLETE)		-	-
100		(OBSOLETE)		-	-
101	prp	ratio of TF coil radial plate area to winding pack area		1.00D-6	0.010D0
102	fimpvar	impurity fraction of element impvar		1.00D-6	0.010D0
103	flhthresh	f-value for L-H power threshold limit equation	15	1.000D0	1.000D6
104	fcwr	f-value for conducting shell radius limit equation	23	0.001D0	1.000D0
105	fnbshinef	f-value for NBI shine-through fraction limit equation	59	0.001D0	1.000D0
106	ftmargoh	f-value for CS coil temperature margin limit equation	60	0.001D0	1.000D0
107	favail	f-value for minimum availability limit equation	61	0.001D0	1.000D0
108	breeder_f	breeder volume ratio: Li4SiO4/(Be12Ti+Li4SiO4)		0.060D0	1.000D0
109	ralpne	thermal alpha density / electron density		0.050D0	0.150D0
110	ftaulimit	f-value for limit on ratio of alpha particle to energy confinement times	62	0.001D0	1.000D0
111	fniterpump	f-value for constraint that number of pumps ¡ tfno	63	0.001D0	1.000D0
112	fzeffmax	f-value for Zeff limit equation	64	0.001D0	1.000D0
113	ftaucq	f-value for quench time limit equation	65	0.001D0	1.000D0
114	fw_channel_length	Length of a single first wall channel	39	0.001D0	1.000D3
115	fpoloidalpower	f-value for max rate of change of energy in poloidal field	66	0.001D0	1.000D0

Table 2.2: *Iteration variables 56 onwards. The f-values correspond to the given constraint equations (see Table 2.3). The other iteration variables are shown in Table 2.1.*

2.5 Constraint Equations

Any computer program naturally contains myriads of equations. The built-in equation solvers within PROCESS act on a special class, known as *constraint equations*, all of which are formulated in routine constraint_eqns in source file constraint_equations.f90. Table 2.3 summarises the constraint equations available in PROCESS. These can be split into two types — (1) consistency equations, that enforce consistency between the physics and engineering parameters, and (2) limit equations, that enforce various parameters to lie within their allowed limits. The neqns constraint equations that the user chooses for a given run are activated by including the equation numbers in the first neqns elements of array icc.

2.5.1 Consistency equations

Consistency equations are *equalities* that ensure that the machine produced by PROCESS is self-consistent. This means, therefore, that many of these constraint equations should *always* be used, namely equations 1, 2, 10 and 11 (see Table 2.3). Equation 7 should also be activated if neutral beam injection is used. The other consistency equations can be activated if required.

A typical consistency equation ensures that two functions g and h are equal:

$$\begin{aligned} g(x, y, z, \ldots) &= h(x, y, z, \ldots) \\ c_i &= 1 - \frac{g}{h} \end{aligned}$$

The equation solvers VMCON and HYBRD need the constraint equations c_i to be given in the form shown, since they adjust the iteration variables so as to obtain $c_i = 0$, thereby ensuring that $g = h$.

2.5.2 Limit equations

The limit equations are *inequalities* that ensure that various physics or engineering limits are not exceeded. Each of these equations has an associated *f-value*, which allow them to be *coded* as equalities. The f-values are used as follows.

In general, limit equations have the form

$$\textit{calculated quantity} = f \times \textit{maximum allowable value}$$

where f is the f-value. In optimisation mode, all iteration variables have prescribed lower and upper bounds. If f is chosen to be an iteration variable and is given a lower bound of zero and an upper bound of one, then the limit equation does indeed constrain the calculated quantity to lie between zero and its maximum allowable value, as required.

As with the consistency equations, the general form of the limit equations is

$$c_i = 1 - f.\frac{h_{\max}}{h}$$

where $h_{\max}$ is the maximum allowed value of the quantity h.

Sometimes, the limit equation and f-value are used to ensure that quantity h is *larger* than its *minimum* value $h_{\min}$. In this case, $0 \leq f \leq 1$ (as before), but the equation takes the form

$$c_i = 1 - f.\frac{h}{h_{\min}}$$

By fixing the f-value (i.e. not including it in the `ixc` array), the limit equations can be used as equality constraints. For example, to set the net electric power to a certain value, the following should be carried out:

1. Activate constraint 16 (net electric power lower limit) by including it in the first `neqns` elements of array `icc`
2. Set the corresponding f-value `fpnetel = 1.0D0`
3. Ensure that `fpnetel` (iteration variable no. 25) *IS NOT* selected as an iteration variable.
4. Set `pnetelin` to the required net electric power.

Limit equations are not restricted to optimisation mode. In non-optimisation mode, the iteration variables are not bounded, but the f-values can still be used to provide information about how calculated values compare with limiting values, without having to change the characteristics of the device being benchmarked to find a solution.

It is for this reason that all the constraint equations used in `PROCESS` are formulated as equalities, despite the fact that equation solver `VMCON` can solve for inequalities as well. The use of f-values precludes this need, and allows the non-optimising equation solver HYBRD to use the same constraint equations.

icc no.	description	type	corresponding ixc variables
1	plasma beta consistency	C	**5**
2	global power balance	C	**10**,1,2,3,4,6,11
3	ion power balance (DEPRECATED - DO NOT USE)	C	**10**,1,2,3,4,6,11
4	electron power balance (DEPRECATED - DO NOT USE)	C	**10**,1,2,3,4,6,11
5	density upper limit	L	**9**,1,2,3,4,5,6
6	epsilon-beta poloidal upper limit	L	**8**,1,2,3,4,6
7	beam ion density (NBI)	C	**7**
8	neutron wall load upper limit	L	**14**,1,2,3,4,6
9	fusion power upper limit	L	**26**,1,2,3,4,6
10	toroidal field 1/R consistency	C	**12**,1,2,3,13
11	radial build consistency	C	**3**,1,13,16,29,42,61
12	volt second capability lower limit	L	**15**,1,2,3
13	burn time lower limit (PULSE)	L	**21**,1,16,17,22,29,42,44,61
14	neutral beam decay lengths = `tbeamin` consistency (NBI)	C	**19**,1,2,3,6
15	L-H power threshold limit	L	**103**
16	net electric power lower limit	L	**25**,1,2,3
17	radiation fraction upper limit	L	**28**
18	divertor heat load upper limit	L	**27**
19	MVA upper limit	L	**30**
20	neutral beam tangency radius upper limit (NBI)	L	**33**,31,3,13
21	minor radius lower limit	L	**32**
22	divertor collisionality upper limit	L	**34**,43
23	conducting shell to plasma minor radius ratio upper limit	L	**104**,1,74
24	Beta upper limit (also beta limit in stellarators)	L	**36**,1,2,3,4,6,18
25	peak toroidal field upper limit	L	**35**,3,13,29
26	central solenoid current density at End of Flat-top upper limit	L	**38**,37,41,12
27	central solenoid current density at Beginning of Pulse upper limit	L	**39**,37,41,12
28	fusion gain Q lower limit	L	**45**,47,40
29	inboard radial build = specified value	C	**3**,1,13,16,29,42,61
30	injection power upper limit	L	**46**,47,11
31	TF coil case stress upper limit (SCTF)	L	**48**,56,57,58,59,60,24
32	TF coil conduit stress upper limit (SCTF)	L	**49**,56,57,58,59,60,24
33	TF coil $I_{\text{operational}}/I_{\text{critical}}$ upper limit (SCTF)	L	**50**,56,57,58,59,60,24
34	TF coil dump voltage upper limit (SCTF)	L	**51**,52,56,57,58,59,60,24
35	TF coil $J_{\text{winding pack}}/J_{\text{protection}}$ upper limit (SCTF)	L	**53**,56,57,58,59,60,24
36	TF coil temperature margin lower limit (SCTF)	L	**54**,55,56,57,58,59,60,24
37	current drive gamma upper limit	L	**40**,47
38	first wall coolant temperature rise upper limit (PULSE)	L	**62**
39	first wall peak temperature upper limit (PULSE)	L	**63**
40	injection power lower limit (PULSE)	L	**64**
41	central solenoid current ramp-up time lower limit (PULSE)	L	**66**,65
42	cycle time lower limit (PULSE)	L	**67**,65,17
43	average centrepost temperature (ST)	C	**69**,70,13
44	peak centrepost temperature upper limit (ST)	L	**68**,69,70
45	edge safety factor lower limit (ST)	L	**71**,1,2,3
46	Ip/Irod upper limit (ST)	L	**72**,2,60
47	TF coil toroidal thickness upper limit (RFP)	L	**76**,77,13,3
48	poloidal beta upper limit	L	**79**,2,3,18
49	reversal parameter < 0 (RFP)	L	**80**,78,3,1
50	IFE repetition rate upper limit (IFE)	L	**86**

Table 2.3: *Summary of the first 50 constraint equations present in* `PROCESS`*. Consistency equations are marked C, limit equations are marked L. Some (non-exhaustive) iteration variable numbers (see Tables 2.1 and 2.2) that directly affect the associated constraint equations are given, the one listed first being the most relevant.*

icc no.	description	type	corresponding ixc variables
51	startup volt-seconds consistency (PULSE)	C	**16**,29,3,1
52	tritium breeding ratio lower limit	L	**89**,90,91
53	peak neutron fluence on TF coil upper limit	L	**92**,93,94
54	peak TF coil nuclear heating upper limit	L	**95**,93,94
55	final He concentration in vacuum vessel upper limit	L	**96**,93,94
56	$P_{\text{separatrix}}/R_{\text{major}}$ upper limit	L	**97**,1,3,102
57	(OBSOLETE) TF coil outer leg toroidal thickness lower limit (SCTF)	L	**99**,29,13
58	(OBSOLETE) TF coil outer leg radial thickness lower limit (SCTF)	L	**100**,13
59	Neutral beam shine-through fraction upper limit (NBI)	L	**105**,6,19,4
60	Central solenoid temperature margin lower limit (SCTF)	L	**106**
61	Minimum availability value limit	L	**107**
62	Lower limit on the ratio of alpha particle to energy confinement times	L	**110**
63	Number of vacuum pumps (vacuum_model=simple)	L	**111**
64	Limit on Zeff $\leq$ Zeffmax	L	**112**
65	TF dump time greater than or equal to calculated quench time	L	**56**, 113
66	Limit on rate of change of energy in poloidal field	L	**65, 115**

Table 2.4: *Summary of constraint equations 51 onwards. Consistency equations are marked C, limit equations are marked L. Some (non-exhaustive) iteration variable numbers (see Tables 2.1 and 2.2) that directly affect the associated constraint equations are given, the one listed first being the most relevant.*

2.6 Figures of Merit

In optimisation mode, `PROCESS` finds the self-consistent set of iteration variable values that maximises or minimises a certain function of them, known as the *figure of merit*. Several possible figures of merit are available, all of which are formulated in routine `FUNFOM` in source file `evaluators.f90`. Switch `minmax` is used to control which figure of merit is to be used, as summarised in Table 2.5. If the figure of merit is to be minimised, `minmax` should be positive, and if a maximised figure of merit is desired, `minmax` should be negative.

2.7 Scanning Variables

One of a number of variables can be scanned during the course of a `PROCESS` run. This option provides a method of determining the sensitivity of the results to different input assumptions. The user specifies which variable is to be scanned (see Table 2.6) and its required value at each point in the scan. Set input parameter `isweep` to the desired number of scan points. The scanned variable to use is defined by the value of `nsweep`, and the chosen variable's values during the scan are set in array `sweep`.

Runs involving scans of this kind can only be performed in optimisation mode. The results from the previous scan point are used as the input to the next scan point. Routine `SCAN` in source file `scan.f90` stores many of the output quantities in a separate output file called `PLOT.DAT`, which can be read by the utility program `plot_sweep` to produce graphical output (see Chapter 6).

It is also possible to scan a derived quantity that is not set directly by the user. For instance, one can scan the net electric power by constraining it to a specified value using the technique described in Section 2.5.2. The required net electric power, `pnetelin`, is then used as the scanning variable.

For obvious reasons, the active scanning variable must not also be an active iteration variable.

`minmax`	description
±1	plasma major radius
±2	not used
±3	neutron wall load
±4	total TF coil + PF coil power
±5	ratio of fusion power to injection power
±6	cost of electricity
±7	$\begin{cases} \text{direct cost} & \text{if } \texttt{ireactor = 0} \\ \text{constructed cost} & \text{otherwise} \end{cases}$
±8	aspect ratio
±9	divertor heat load
±10	toroidal field on axis
±11	injection power
±12	hydrogen plant capital cost
±13	hydrogen production rate
±14	pulse length
±15	plant availability factor (N.B. requires `iavail>=1`)
±16	minimise R0 and maximise burn time (linear combination)
±17	net electrical power

Table 2.5: *Summary of the available figures of merit in* ***PROCESS****. If the figure of merit is to be minimised,* ***minmax*** *should be positive, and if a maximised figure of merit is desired,* ***minmax*** *should be negative.*

`nsweep`	scan variable	description
1	`aspect`	plasma aspect ratio
2	`hldivlim`	maximum divertor heat load
3	`pnetelin`	required net electric power
4	`hfact`	confinement time H-factor
5	`oacdcp`	overall current density in TF coil inboard leg
6	`walalw`	allowable wall load
7	`beamfus0`	beam-background fusion multiplier
8	`fqval`	f-value for fusion gain limit eqn
9	`te`	electron temperature
10	`boundu(15)`	upper bound on f-value `fvs`
11	`dnbeta`	beta g coefficient
12	`bscfmax`	bootstrap current fraction (use negative values)
13	`boundu(10)`	upper bound on confinement time H-factor `hfact`
14	`fiooic`	f-value for TF coil operational current limit eqn
15	`fjprot`	f-value for TF coil current protection limit eqn
16	`rmajor`	plasma major radius
17	`bmxlim`	maximum toroidal field
18	`gammax`	maximum current drive gamma
19	`boundl(16)`	lower bound on central solenoid thickness `ohcth`
20	`tbrnmn`	minimum burn time (pulsed operation machine)
21	`sigpfalw`	allowable stress in the PF coils
22	`cfactr`	plant availability factor (N.B. requires `iavail=0`)
23	`boundu(72)`	upper bound on f-value `fipir`
24	`powfmax`	maximum fusion power
25	`kappa`	plasma elongation
26	`triang`	plasma triangularity
27	`tbrmin`	minimum tritium breeding ratio (`blktmodel=1`)
28	`bt`	toroidal field on axis
29	`coreradius`	normalised radius defining the core region
30	`fimpvar`	impurity fraction of element `impvar`
31	`taulimit`	Taup/taueff lower limit

Table 2.6: *Summary of the scanning variables available in* `PROCESS`.

Chapter 3

Physics, Engineering and Other Models

There are a great number of individual models within PROCESS, characterising many different aspects of a fusion power plant. Several of these will always be used by the code and so require no input by the user to activate them. However, in many cases there is a choice of model available, and each of these has its own user-controlled switches or flags. This chapter summarises some of these models, and indicates their location and interaction within the code, together with the relevant switch settings and required parameter values. The concepts used (iteration variables, constraint equations, etc.), and instructions on how to set switches, etc., are explained fully in Chapter 2.

It is essential for the user to refer to the variable descriptor file, `vardes.html`, this contains details of all the parameters within the code that can be changed by the user, in order to customise the machine modelled by PROCESS.

Disclaimer: Users are discouraged from using non-default or older models, as they are likely to be less well tested than the default models and should therefore be treated with caution.

3.1 Tokamak Power Plant

The default (and most detailed) power plant model in PROCESS is based on the tokamak magnetic-confinement fusion concept. This section describes the models relevant to such a plant in some detail, starting with the plasma at the centre of the fusion power core, and moving outwards to the external components, power subsystems and buildings. However, many of these models are also partly or wholly relevant for the other available machine types, especially outside the fusion power core. The specific details for these alternative models are introduced later in the Chapter.

3.1.1 Radial and vertical build

Figure 3.1 shows schematically the layout of a typical tokamak as modelled by PROCESS. This is the so-called 'build' of the machine — the relative locations of the major components. Their positions are referenced to the (R, Z) coordinate system, where R is the radial distance from the vertical centreline (axis) of the torus, and Z is the vertical distance from the equatorial midplane, about which the machine is assumed to be up-down symmetrical (by default; the vertical build is slightly different for single null plasma devices — see Figure 3.3). Components are often referred to as being 'inboard' or 'outboard', which simply means that they lie at a radius R less than or greater than R_0, respectively, where R_0 is the plasma major radius (`rmajor`). For the sake of clarity the thicknesses are not drawn

to scale, and the space labelled as the divertor does not indicate in any way the actual shape of that component.

The first wall, blanket, shield and vacuum vessel may be either D-shaped in cross-section, or each may be defined by two half-ellipses; compare their shapes in Figures 3.1 and 3.2. The choice between these two possibilities is set using input parameter `fwbsshape` [8], which should be `1` for D-shaped, or `2` for ellipses.

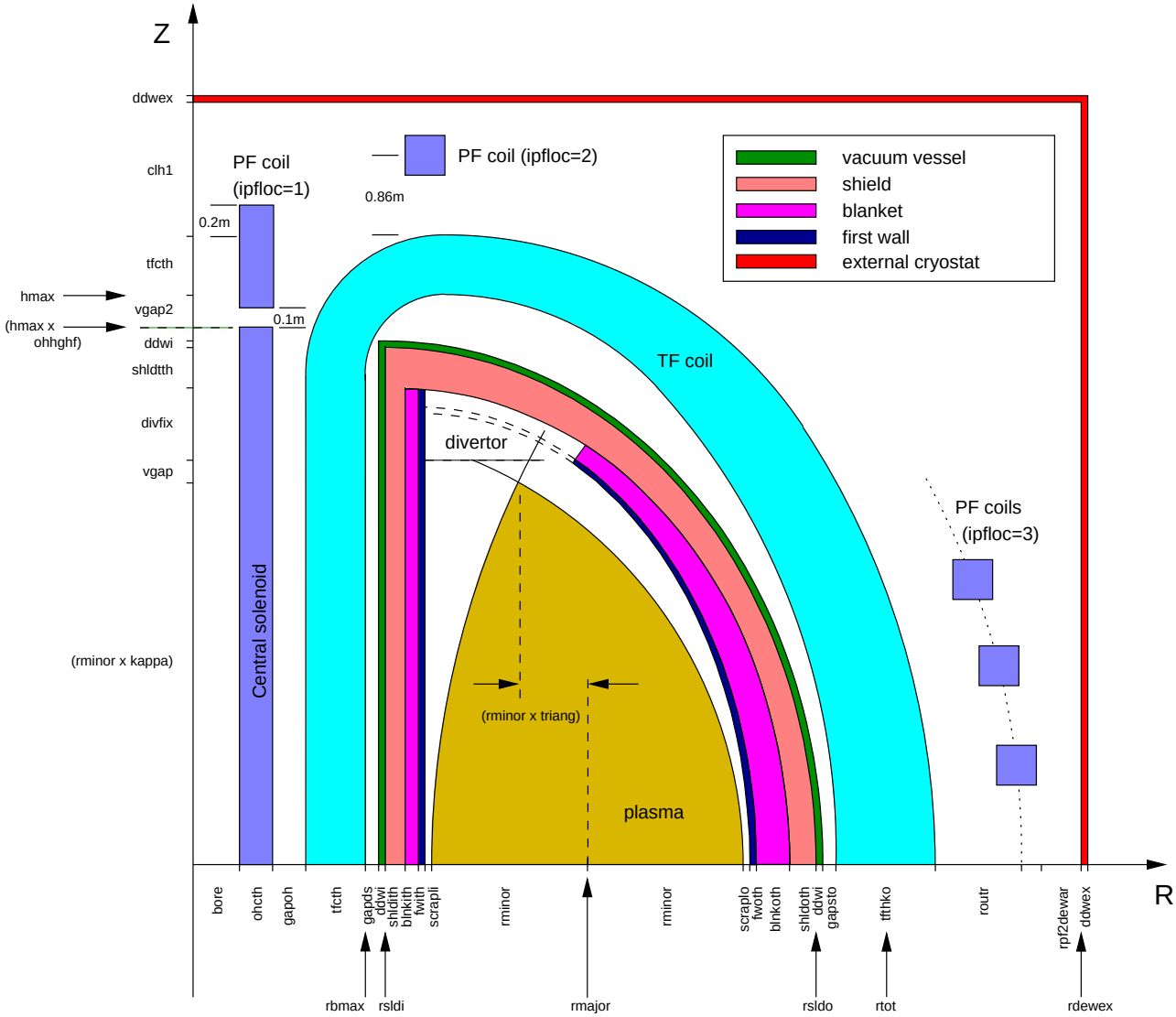


Figure 3.1: *Schematic diagram of the fusion power core of a typical tokamak power plant modelled by* ***PROCESS****, showing the relative positions of the components. A double null plasma is assumed (****snull=0****) — compare Figure 3.3, and the first wall, blanket, shield and vacuum vessel are D-shaped in cross-section (chosen by setting switch* ***fwbsshape=1****) — compare Figure 3.2. Also shown are the code variables used to define the thicknesses of the components. The arrowed labels adjacent to the axes are the total 'builds' to that point. The precise locations and sizes of the PF coils are calculated within the code (see Section 3.1.7).*

Most of the thicknesses shown in Figures 3.1 and 3.2 are input parameters, so are not changed during the course of the simulation. The rest are calculated by the code during execution. In addition, some of the component sizes can be used as *iteration variables* (see Section 2.4) to help in the optimisation

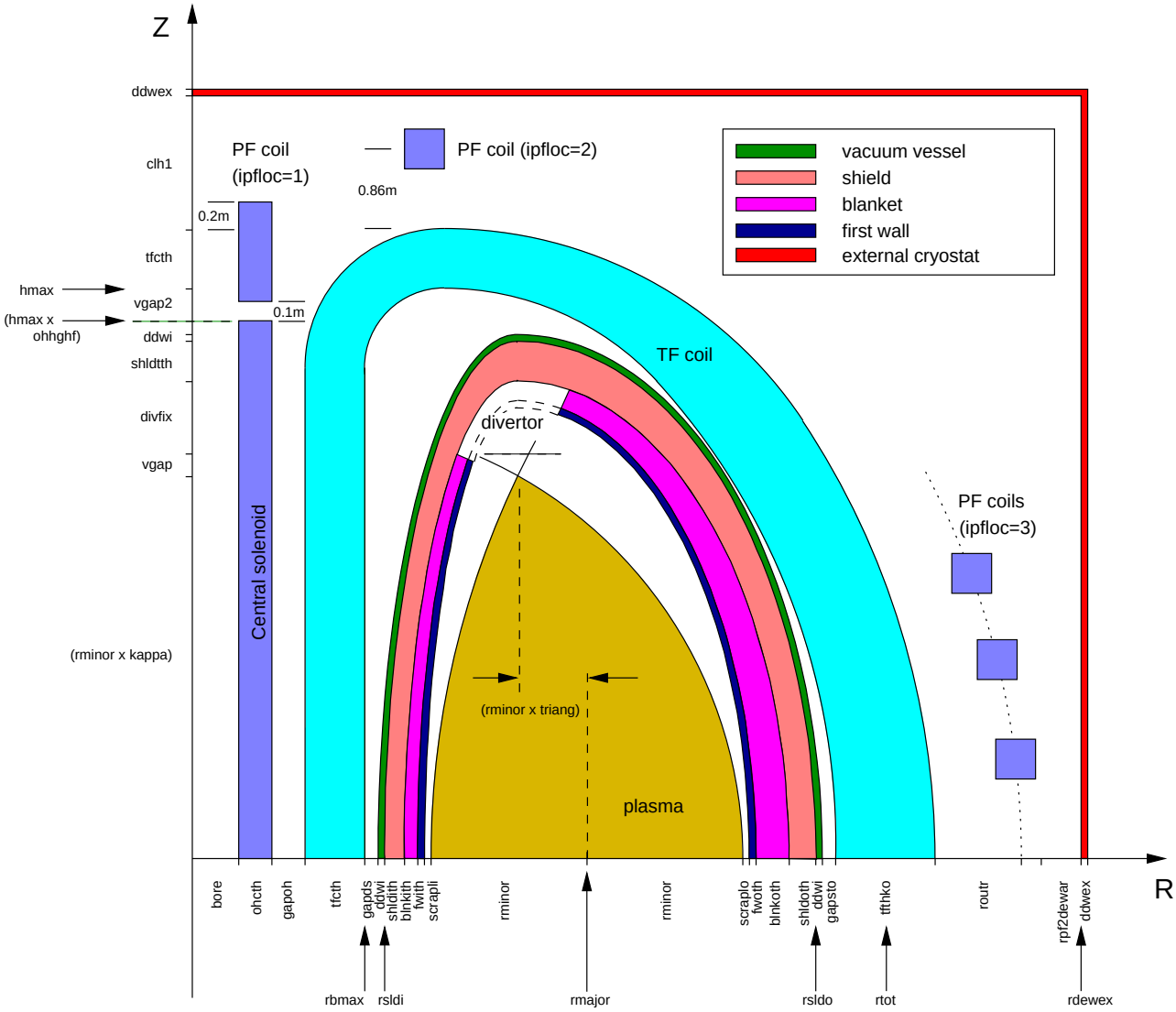


Figure 3.2: *Schematic diagram of the fusion power core of a typical tokamak power plant modelled by* `PROCESS`*. The first wall, blanket, shield and vacuum vessel cross-sectional shapes are each assumed to be defined by two ellipses (chosen by setting switch* `fwbsshape=2`*) — compare Figure 3.1.*

process.

3.1.2 Plasma physics models

By default, the plasma is assumed to have an up-down asymmetric, single null configuration (although this can be changed if desired — see Section 3.1.5). A great number of physics models are coded within PROCESS to describe the behaviour of the plasma parameters such as its current, temperature, density, pressure, confinement etc., and also the various limits that define the stable operating domain.

3.1.2.1 Plasma geometry

The plasma (geometric) major radius R_0 (rmajor) and aspect ratio A (aspect) define the size of the plasma torus. The plasma minor radius a (rminor) is calculated from these values. The shape of the plasma cross-section is given by its last closed flux surface (LCFS) elongation κ (kappa) and triangularity δ (triang), which can be scaled automatically with the aspect ratio if required using switch ishape:

- If ishape = 0, the input values for kappa and triang are used directly.
- If ishape = 1, the following scaling is used, which is suitable for low aspect ratio machines ($\epsilon = 1/A$) [2]:

$$\kappa = 2.05\,(1 + 0.44\,\epsilon^{2.1}) \tag{3.1}$$
$$\delta = 0.53\,(1 + 0.77\,\epsilon^{3}) \tag{3.2}$$

- If ishape = 2, the Zohm ITER scaling [9] is used to calculate the elongation:

$$\kappa = F_{kz} \times \text{minimum}\left(2.0,\ 1.5 + \frac{0.5}{A-1}\right) \tag{3.3}$$

  where input variable fkzohm $= F_{kz}$ may be used to adjust the scaling, while the input value of the triangularity is used unchanged.

If ishape = 0, 1 or 2, the values for the plasma shaping parameters at the 95% flux surface are calculated as follows [10]:

$$\kappa_{95} = \kappa/1.12 \tag{3.4}$$
$$\delta_{95} = \delta/1.5 \tag{3.5}$$

- If ishape = 3, the Zohm ITER scaling [9] is used to calculate the elongation (as for ishape = 2 above), but the triangularity at the 95% flux surface is input via variable triang95, and the LCFS triangularity triang is calculated from it, rather than the other way round.
- Finally, if ishape = 4, the 95% flux surface values kappa95 and triang95 are both used as inputs, and the LCFS values are calculated from them by inverting Equations 3.4 and 3.5.

A constraint relating to the plasma's vertical stability may be turned on if required. In principle, the inner surface of the outboard shield could be used as the location of a conducting shell which should mitigate the vertical displacement growth rate of plasmas with significant elongation [11]. The maximum distance $r_{\text{shell, max}}$ of this shell from the centre of the plasma may be set using input

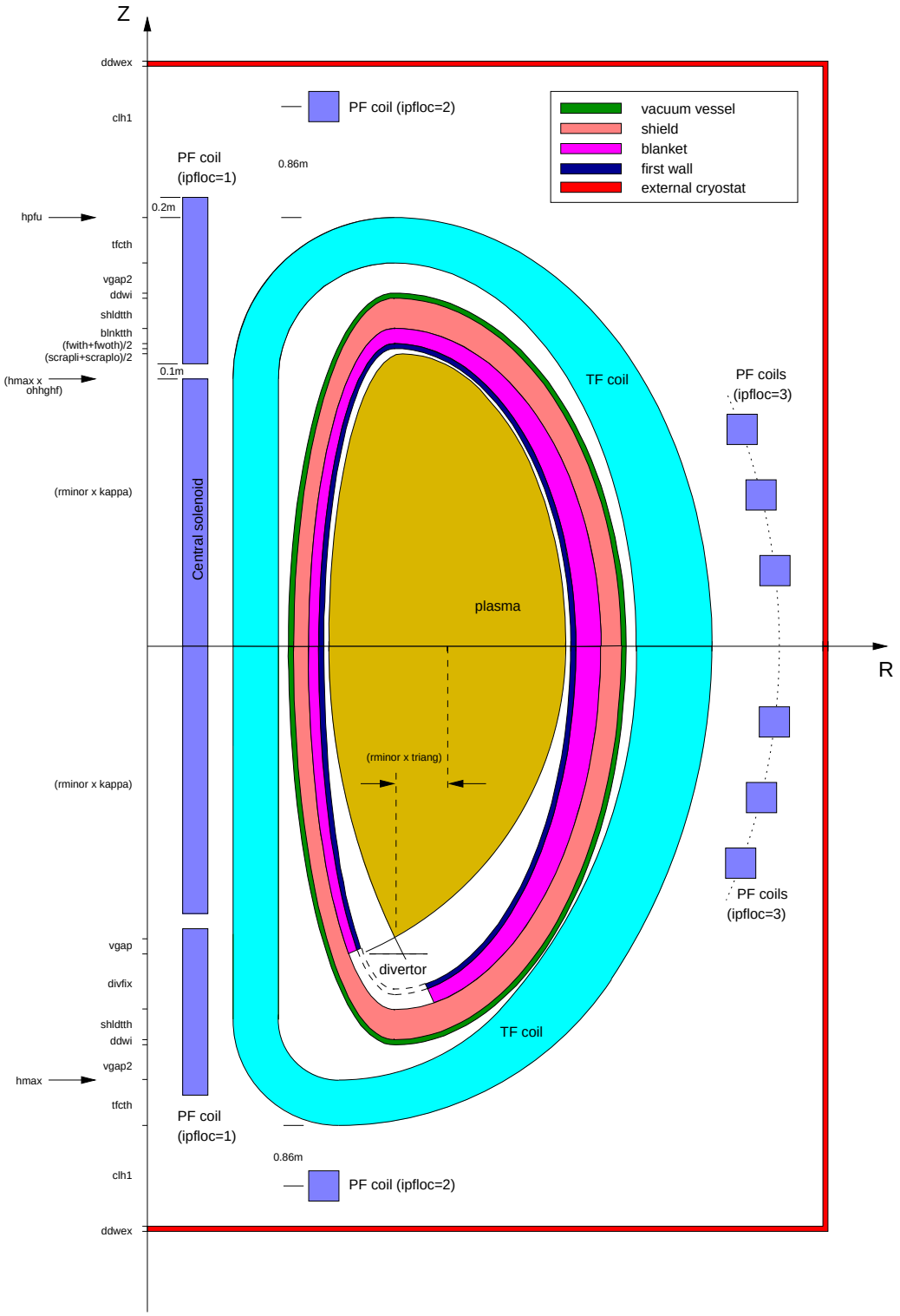


Figure 3.3: *Schematic diagram of the fusion power core of a typical tokamak power plant modelled by* `PROCESS`*, showing the relative positions of the components. A single null plasma is assumed (*`snull=1`*) — compare Figure 3.2. The radial build is the same as for a double null configuration; shown along the vertical axis are the code variables used to define the vertical thicknesses of the components. The arrowed labels adjacent to the axis are the total 'builds' (distance from the midplane, Z=0) to that point. The precise locations and sizes of the PF coils are calculated within the code (see Section 3.1.7).*

parameter `cwrmax`, such that $r_{\text{shell, max}}$ = `cwrmax*rminor`. Constraint equation no. 23 should be turned on with iteration variable no. 104 (`fcwr`) to enforce this. (A scaling of `cwrmax` with elongation should be available shortly.)

The plasma surface area, cross-sectional area and volume are calculated using formulations that approximate the LCFS as a revolution of two arcs which intersect the plasma X-points and the plasma midplane outer and inner radii. (This is a reasonable assumption for double-null diverted plasmas, but will be inaccurate for single-null plasmas, `snull = 1`.) Switch `igeom` determines whether an old method is used (`igeom = 0`) or calculations based on a more recent derivation (`igeom = 1`) [12].

3.1.2.2 Fusion reactions

The most likely fusion reaction to be utilised in a power plant is the deuterium-tritium reaction:

$$\mathrm{D} + \mathrm{T} \Longrightarrow {}^4\mathrm{He} + \mathrm{n} + 17.6\,\mathrm{MeV} \tag{3.6}$$

20% of the energy produced is given to the alpha particles (^{4}He), a fraction of which remain (c.f. `falpha`, Section sec:corepower) within the plasma and thermalise (slow down) due to collisions, thus heating the plasma. The remaining 80% is carried away by the neutrons, which deposit their energy within the blanket and shield.

`PROCESS` can also model D-^{3}He power plants, which utilise the following primary fusion reaction:

$$\mathrm{D} + {}^3\mathrm{He} \Longrightarrow {}^4\mathrm{He} + \mathrm{p} + 18.3\,\mathrm{MeV} \tag{3.7}$$

The fusion reaction rate is significantly different to that for D-T fusion, and the power flow from the plasma is modified since charged particles are produced rather than neutrons. Because only charged particles (which remain in the plasma) are produced by this reaction, the whole of the fusion power is used to heat the plasma. Useful energy is extracted from the plasma since the radiation power produced is very high, and this can be converted to electricity in a number of ways.

Since the temperature required to ignite the D-^{3}He reaction is considerably higher than that for D-T, it is necessary to take into account the following D-D reactions, which have significant reaction rates at such temperatures:

$$\mathrm{D} + \mathrm{D} \Longrightarrow {}^3\mathrm{He} + \mathrm{n} + 3.27\,\mathrm{MeV} \tag{3.8}$$

$$\mathrm{D} + \mathrm{D} \Longrightarrow \mathrm{T} + \mathrm{p} + 4.03\,\mathrm{MeV} \tag{3.9}$$

Also, as tritium is produced by the latter reaction, D-T fusion is also possible. As a result, there is still a small amount of neutron power extracted from the plasma.

Pure D-^{3}He tokamak power plants do not include blankets, because of the near absence of neutrons leaving the plasma, and the fact that no tritium needs to be produced for fuel.

The contributions from all four of the above fusion reactions are included in the total fusion power production calculation. The fusion reaction rates are calculated using the parametrizations in [13], integrated over the plasma profiles (correctly, with or without pedestals).

The fractional composition of the "fuel" ions (D, T and ^{3}He) is controlled using the three variables `fdeut`, `ftrit` and `fhe3`, respectively:

$$\begin{aligned} n_{\text{fuel}} &= n_D + n_T + n_{^3\text{He}} \quad \text{particles/m}^3 \\ n_D &= \texttt{fdeut}\, n_{\text{fuel}} \\ n_T &= \texttt{ftrit}\, n_{\text{fuel}} \\ n_{^3\text{He}} &= \texttt{fhe3}\, n_{\text{fuel}} \end{aligned}$$

`PROCESS` checks that `fdeut + ftrit + fhe3 = 1.0`, and stops with an error message otherwise.

3.1.2.3 Plasma profiles

If switch `ipedestal = 0`, the plasma profiles are assumed to be parabolic, i.e. they are of the form

$$\text{Density}: n(\rho) = n_0 \left(1-\rho^2\right)^{\alpha_n} \tag{3.10}$$

$$\text{Temperature}: T(\rho) = T_0 \left(1-\rho^2\right)^{\alpha_T} \tag{3.11}$$

$$\text{Current}: J(r) = J_0 \left(1-\rho^2\right)^{\alpha_J} \tag{3.12}$$

where $\rho = r/a$, and a is the plasma minor radius. This gives volume-averaged values $\langle n\rangle = n_0/(1+\alpha_n)$, and line-averaged values $\bar{n} \sim n_0/\sqrt{(1+\alpha_n)}$, etc. These volume- and line-averages are used throughout the code along with the profile indices α, in the various physics models, many of which are fits to theory-based or empirical scalings. Thus, the plasma model in `PROCESS` may be described as "$\frac{1}{2}$-D". The relevant profile index variables are `alphan`, `alphat` and `alphaj`, respectively (see Section 3.1.2.9).

However, by default, `ipedestal = 1` which allows the density and temperature profiles to include a pedestal, using the forms specified in [14]:

$$\text{density:} \qquad n(\rho) = \begin{cases} n_{ped} + (n_0 - n_{ped})\left(1 - \dfrac{\rho^2}{\rho_{ped,n}^2}\right)^{\alpha_n} & 0 \le \rho \le \rho_{ped,n} \\ n_{sep} + (n_{ped} - n_{sep})\left(\dfrac{1-\rho}{1-\rho_{ped,n}}\right) & \rho_{ped,n} < \rho \le 1 \end{cases} \tag{3.13}$$

$$\text{temperature:} \qquad T(\rho) = \begin{cases} T_{ped} + (T_0 - T_{ped})\left(1 - \dfrac{\rho^{\beta_T}}{\rho_{ped,T}^{\beta_T}}\right)^{\alpha_T} & 0 \le \rho \le \rho_{ped,T} \\ T_{sep} + (T_{ped} - T_{sep})\left(\dfrac{1-\rho}{1-\rho_{ped,T}}\right) & \rho_{ped,T} < \rho \le 1 \end{cases} \tag{3.14}$$

Subscripts 0, *ped* and *sep*, denote values at the centre ($\rho = 0$), the pedestal ($\rho = \rho_{ped}$) and the separatrix ($\rho = 1$), respectively. The density and temperature peaking parameters α_n and a α_T as well as the second exponent β_T (input parameter `tbeta`, not to be confused with the plasma beta) in the temperature profile can be chosen by the user, as can the pedestal heights and the values at the separatrix (`neped, nesep` for the electron density, and `teped, tesep` for the electron temperature; the ion equivalents are scaled from the electron values by the ratio of the volume-averaged values). The density at the centre is given by

$$\begin{aligned} n_0 = \; & \frac{1}{3\rho_{ped,n}^2}\left[3\langle n\rangle(1+\alpha_n) + n_{sep}(1+\alpha_n)(-2+\rho_{ped,n}+\rho_{ped,n}^2)\right. \\ & \left. -n_{ped}\left((1+\alpha_n)(1+\rho_{ped,n}) + (\alpha_n - 2)\rho_{ped,n}^2\right)\right] \end{aligned} \tag{3.15}$$

where $\langle n\rangle$ is the volume-averaged density. The temperature at the centre is given by

$$T_0 = T_{ped} + \gamma\left[T_{ped}\,\rho_{ped,T}^2 - \langle T\rangle + \frac{1}{3}(1-\rho_{ped,T})\left[(1+2\rho_{ped,T})\,T_{ped} + (2+\rho_{ped,T})\,T_{sep}\right]\right] \tag{3.16}$$

with

$$\gamma = \begin{cases} \dfrac{-\Gamma(1+\alpha_T+2/\beta_T)}{\rho_{ped,T}^2\,\Gamma(1+\alpha_T)\,\Gamma((2+\beta_T)/\beta_T)} & \text{for integer } \alpha_T \\ \dfrac{\Gamma(-\alpha_T)\sin(\pi\alpha)\,\Gamma(1+\alpha_T+2/\beta_T)}{\pi\rho_{ped,T}^2\,\Gamma((2+\beta_T)/\beta_T)} & \text{for non-integer } \alpha_T \end{cases} \tag{3.17}$$

where Γ is the gamma function.

Note that density and temperature can have different pedestal positions $\rho_{ped,n}$ (`rhopedn`) and $\rho_{ped,T}$ (`rhopedt`) in agreement with simulations.

The pedestal density can be set directly (if `iscdens=1`), or as a fraction of the Greenwald density (if `iscdens=1`). The default fraction is 0.8 [15].

3.1.2.4 Beta limits

The plasma beta limit [16, 17] is given by

$$\langle\beta\rangle < g\,\frac{I(\mathrm{MA})}{a(\mathrm{m})\,B_0(\mathrm{T})} \tag{3.18}$$

where B_0 is the axial vacuum toroidal field, and β is defined with respect to the total equilibrium **B**-field [17]. The beta coefficient g is set using input parameter `dnbeta` (but see Section 3.1.2.9). To apply the beta limit, constraint equation no. 24 should be turned on with iteration variable no. 36 (`fbetatry`). The limit can be applied to either the total plasma beta, in which case switch `iculbl` should be set to 0, to only the thermal component of the plasma beta, in which case `iculbl` should be set to 1, or to the thermal plus neutral beam components, in which case `iculbl` should be set to 2.

Aspect ratio scaling of beta g coefficient

Switch `gtscale` determines whether the beta g coefficient `dnbeta` should scale with aspect ratio (`gtscale` $\neq$ `0`), or be fixed at the input value (`gtscale = 0`). Note that `gtscale` is over-ridden if `iprofile = 1` (see Section 3.1.2.9).

Limiting $\epsilon.\beta_p$

To apply a limit to the value of $\epsilon.\beta_p$, where $\epsilon = a/R$ is the inverse aspect ratio, constraint equation no. 6 should be turned on with iteration variable no. 8 (`fbeta`). The limiting value of $\epsilon.\beta_p$ should be set using input parameter `epbetmax`.

3.1.2.5 Fast alpha pressure contribution

Switch `ifalphap` may be used to select the model used to calculate the pressure contribution from the fast alpha particles:

$$\frac{\beta_\alpha}{\beta_{th}} = 0.29\,(\langle T_{10}\rangle - 0.37)\left(\frac{n_{DT}}{n_e}\right)^2 \qquad \texttt{ifalphap = 0}\ [16] \tag{3.19}$$

$$\frac{\beta_\alpha}{\beta_{th}} = 0.26\,(\langle T_{10}\rangle - 0.65)^{0.5}\left(\frac{n_{DT}}{n_e}\right)^2 \qquad \texttt{ifalphap = 1}\ \text{(default)}\ [18] \tag{3.20}$$

The latter model is a better estimate at higher temperatures.

3.1.2.6 Density limits

Several density limit models [17] are available in `PROCESS`. These are calculated in routine `CULDLM`, which is called by `PHYSICS`. To enforce any of these limits, turn on constraint equation no. 5 with iteration variable no. 9 (`fdene`). In addition, switch `idensl` must be set to the relevant value, as follows:-

`idensl = 1 :` ASDEX model

`idensl = 2 :` Borrass model for ITER, I

`idensl = 3 :` Borrass model for ITER, II

`idensl = 4 :` JET edge radiation model

`idensl = 5 :` JET simplified model

`idensl = 6 :` Hugill-Murakami $M.q$ model

`idensl = 7 :` Greenwald model

3.1.2.7 Impurities and radiation

The impurity radiation model in `PROCESS` can be chosen using the switch `imprad_model`, where `imprad_model = 0` gives the original ITER 1989 model [19], and `imprad_model = 1` uses a multi-impurity model which integrates the radiation contributions over an arbitrary choice of density and temperature profiles [22].

If `imprad_model = 0`, the impurity species and fractions are chosen using input parameters `impc`, `impo`, `fbfe`, `cfe0` and `zfear`; see the variable descriptor file for more details.

If `imprad_model = 1`, the impurity number density fractions relative to the electron density are set using input array `fimp(1 to nimp)`, where `nimp = 14` is the number of impurity species in the radiation model. The available impurities are as follows:

1. Hydrogen (fraction calculated by code)
2. Helium (fraction calculated by code)
3. Beryllium
4. Carbon
5. Nitrogen
6. Oxygen
7. Neon
8. Silicon
9. Argon
10. Iron
11. Nickel
12. Krypton
13. Xenon
14. Tungsten

As stated above, the number density fractions for hydrogen (all isotopes) and helium need not be set, as they are calculated by the code to ensure that plasma quasi-neutrality is maintained, and taking into account the fuel ratios `fdeut`, `ftrit` and `fhe3` (see Section 3.1.2.2), and the alpha particle fraction `ralpne` which may be input by the user.

The impurity fraction of one of the elements listed in array `fimp` may be used as an iteration variable (although it will only have any effect if `imprad_model = 1`). The element to use is specified using input parameter `impvar`, which may be set to a value between 3 and `nimp`, and the initial estimate to use for the element's impurity fraction must be set using iteration variable no. 102 (`fimpvar`).

The synchrotron radiation power [23, 24] is assumed to originate from the plasma core. The wall reflection factor `ssync` may be set by the user.

By changing the input parameter `coreradius`, the user may set the normalised radius defining the core region (`imprad_model = 1` only). Only the impurity and synchrotron radiation from the core region affects the confinement scaling (but see the `iradloss` description in Section 3.1.2.10). Figure 3.4 elucidates the radiation power contributions, while Figures 3.5 and **??** show how the radiation power propagates through the fusion power core.

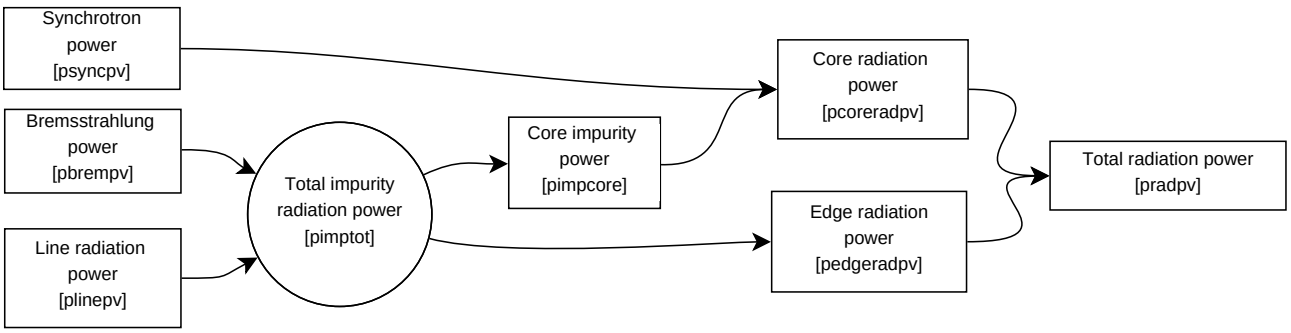


Figure 3.4: *Schematic diagram of the radiation power contributions and how they are split between core and edge radiation, for `imprad_model = 1`.*

Constraint equation no. 17 with iteration variable no. 28 (`fradpwr`) ensures that the calculated total radiation power does not exceed the total power available that can be converted to radiation (i.e. the sum of the fusion alpha power, other charged particle fusion power, auxiliary injected power and the ohmic power). This constraint should always be turned on.

3.1.2.8 Plasma current scaling laws

A number of plasma current scaling laws exploiting the inverse relationship between plasma current and edge safety factor q_ψ [17] are available in `PROCESS`. These are calculated in routine `CULCUR`, which is called by `PHYSICS`. Flag `icurr` must be set to the relevant value, as follows:-

`icurr = 1 :` Peng analytic fit

`icurr = 2 :` Peng double null divertor scaling (ST) [2]

`icurr = 3 :` Simple ITER scaling

`icurr = 4 :` Revised ITER scaling [25]

`icurr = 5 :` Todd empirical scaling, I

`icurr = 6 :` Todd empirical scaling, II

`icurr = 7 :` Connor-Hastie model

3.1.2.9 Plasma current profile consistency

Self-consistency between the plasma current profile parameters [10] can be enforced by setting switch `iprofile` to 1. This ensures that the current profile peaking factor `alphaj` is consistent with the input values for the safety factor on axis and at the plasma edge (`q0` and `q`, respectively), the plasma internal inductance l_i is consistent with this `alphaj`, and the beta g coefficient `dnbeta` scales with l_i.

It is recommended that current scaling law `icurr = 4` is used if `iprofile = 1`. Switch `gtscale` is over-ridden if `iprofile = 1`.

3.1.2.10 Confinement time scaling laws

The particle transport loss power in Watts/m^3 from the plasma is defined as

$$P_{\text{loss}} = \frac{W}{\tau_E} \tag{3.21}$$

where the plasma stored energy per unit volume W is given by

$$W = \frac{3}{2}\, n\, e\, T$$

with particle number density n in m^{-3} and particle temperature T in eV. `PROCESS` assumes that the electron and ion energy confinement times τ_E are equal.

Many energy confinement time scaling laws are present within `PROCESS`, for tokamaks, RFPs or stellarators. These are calculated in routine `PCOND`. The value of `isc` determines which of the scalings is used in the plasma energy balance calculation (Section 3.1.2.11). Table 3.1 summarises the available scaling laws. The most commonly used is the so-called IPB98(y,2) scaling.

Effect of radiation on energy confinement

Published confinement scalings are all based on low radiation pulses. A power plant will certainly be a high radiation machine — both in the core, due to bremsstrahlung and synchrotron radiation, and in the edge due to impurity seeding. The scaling data do not predict this radiation — that needs to be done by the radiation model. However, if the transport is very "stiff", as predicted by some models, then the additional radiation causes an almost equal drop in power transported by ions and electrons, leaving the confinement nearly unchanged.

To allow for these uncertainties, three options are available, using the switch `iradloss`. In each case, the particle transport loss power P_{loss} (Equation 3.21), referred to in the code as `pscaling`, is derived directly from the energy confinement scaling law (see 3.1.2.10 and Figure 3.4 above).

`iradloss = 0`: Total power lost is scaling power plus radiation:

```
pscaling + pradpv = falpha*palppv + pchargepv + pohmpv + pinjmw/vol
```

`iradloss = 1`: Total power lost is scaling power plus core radiation only:

```
pscaling + pcoreradpv = falpha*palppv + pchargepv + pohmpv + pinjmw/vol
```

isc	scaling law	reference
1	Neo-Alcator (ohmic)	[16]
2	Mirnov (H-mode)	[16]
3	Merezhkin-Muhkovatov (L-mode)	[16]
4	Shimomura (H-mode)	JAERI-M 87-080 (1987)
5	Kaye-Goldston (L-mode)	Nuclear Fusion **25** (1985) p.65
6	ITER 89-P (L-mode)	Nuclear Fusion **30** (1990) p.1999
7	ITER 89-O (L-mode)	[16]
8	Rebut-Lallia (L-mode)	Plasma Physics and Controlled Nuclear Fusion Research **2** (1987) p. 187
9	Goldston (L-mode)	Plas. Phys. Controlled Fusion **26** (1984) p.87
10	T10 (L-mode)	[16]
11	JAERI-88 (L-mode)	JAERI-M 88-068 (1988)
12	Kaye-Big Complex (L-mode)	Phys. Fluids B **2** (1990) p.2926
13	ITER H90-P (H-mode)	
14	ITER Mix (minimum of 6 and 7)	
15	Riedel (L-mode)	
16	Christiansen et al. (L-mode)	JET Report JET-P (1991) 03
17	Lackner-Gottardi (L-mode)	Nuclear Fusion **30** (1990) p.767
18	Neo-Kaye (L-mode)	[16]
19	Riedel (H-mode)	
20	ITER H90-P (amended)	Nuclear Fusion **32** (1992) p.318
21	Large Helical Device (stellarator)	Nuclear Fusion **30** (1990) p.11
22	Gyro-reduced Bohm (stellarator)	Bull. Am. Phys. Society, **34** (1989) p.1964
23	Lackner-Gottardi (stellarator)	Nuclear Fusion **30** (1990) p.767
24	ITER-93H (H-mode)	Plasma Physics and Controlled Nuclear Fusion Research (Proc. 15th Int. Conf., Seville, 1994) IAEA-CN-60/E-P-3
25	TITAN (RFP)	TITAN RFP Fusion Reactor Study, Scoping Phase Report UCLA-PPG-1100, page 5–9, Jan 1987
26	ITER H-97P ELM-free (H-mode)	J. G. Cordey et al., EPS Berchtesgaden, 1997
27	ITER H-97P ELMy (H-mode)	J. G. Cordey et al., EPS Berchtesgaden, 1997
28	ITER-96P (= ITER97-L) (L-mode)	Nuclear Fusion **37** (1997) p.1303
29	Valovic modified ELMy (H-mode)	
30	Kaye PPPL April 98 (L-mode)	
31	ITERH-PB98P(y) (H-mode)	
32	IPB98(y) (H-mode)	Nuclear Fusion **39** (1999) p.2175
33	IPB98(y,1) (H-mode)	Nuclear Fusion **39** (1999) p.2175
34	IPB98(y,2) (H-mode)	Nuclear Fusion **39** (1999) p.2175
35	IPB98(y,3) (H-mode)	Nuclear Fusion **39** (1999) p.2175
36	IPB98(y,4) (H-mode)	Nuclear Fusion **39** (1999) p.2175
37	ISS95 (stellarator)	Nuclear Fusion **36** (1996) p.1063
38	ISS04 (stellarator)	Nuclear Fusion **45** (2005) p.1684
39	DS03 (H-mode)	Plasma Phys. Control. Fusion **50** (2008) 043001, equation 4.13
40	Non-power law	A. Murari et al 2015 Nucl. Fusion 55 073009, doi:10.1088/0029-5515/55/7/073009 Table 4.

Table 3.1: *Summary of the energy confinement time scaling laws in* PROCESS.

`iradloss = 2`: Total power lost is scaling power only, with no additional allowance for radiation. This is not recommended for power plant models.

```
pscaling = falpha*palppv + pchargepv + pohmpv + pinjmw/vol
```

3.1.2.11 Plasma core power balance

Figure 3.5 shows the flow of power as calculated by the code. (Figure 3.9 shows an alternative view of the power transfer outside the reactor core.)

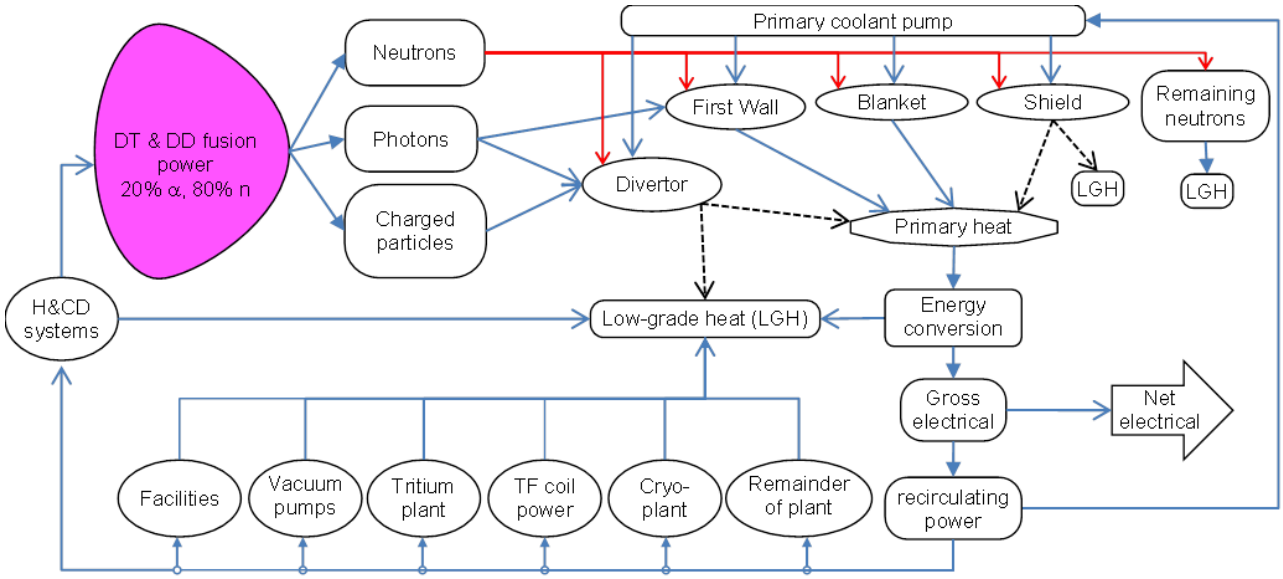


Figure 3.5: *Power flows*

The primary sources of power are the fusion reactions themselves, ohmic power due to resistive heating within the plasma, and any auxiliary power provided for heating and current drive (see Section 3.1.9). The power carried by the fusion-generated neutrons is lost from the plasma, but is deposited in the surrounding material (see Section 3.1.12). A fraction `falpha` of the alpha particle power is assumed to stay within the plasma core to contribute to the plasma power balance. The sum of this core alpha power, any power carried by non-alpha charged particles, the ohmic power and any injected power, is converted into charged particle transport power (P_{loss} in Equation 3.21) plus core radiation power (see Section 3.1.2.7), as shown in Figure 3.5.

The core power balance calculation is turned on using constraint equation no. 2 (which should therefore always be used).

3.1.2.12 Bootstrap current scalings

The fraction of the plasma current provided by the so-called bootstrap effect can be either input into the code directly, or calculated using one of four methods, as summarised here. Note that methods `ibss = 1` to `3` use fits to parabolic density and temperature profiles, and do not take into account the existence of pedestals (`ipedestal = 1`), whereas the Sauter et al. scaling (`ibss = 4`) allows general profiles to be used.

- Direct input: To input the bootstrap current fraction directly, set `bscfmax` to (-1) times the required value.

- ITER scaling [16]: To use the ITER scaling method for the bootstrap current fraction, set `ibss = 1`, and `bscfmax` to the maximum required bootstrap current fraction (≤ 1). This method is valid at high aspect ratio only.
- General scaling [26]: To use a more general scaling method, set `ibss = 2`, and `bscfmax` to the maximum required bootstrap current fraction (≤ 1).
- Numerically fitted scaling [27]: To use a numerically fitted scaling method, valid for all aspect ratios, set `ibss = 3`, and `bscfmax` to the maximum required bootstrap current fraction (≤ 1).
- Sauter, Angioni and Lin-Liu scaling [28, 29]: Set `ibss = 4`, and `bscfmax` to the maximum required bootstrap current fraction (≤ 1).

3.1.2.13 L-H power threshold scalings

Transitions from a standard confinement mode (L-mode) to an improved confinement regime (H-mode), called L-H transitions, are observed in most tokamaks. A range of scaling laws are available that provide estimates of the auxiliary power required to initiate these transitions, via extrapolations from present-day devices. `PROCESS` calculates these power threshold values for the scaling laws listed in Table 3.2, in routine `PTHRESH`.

To enforce one of these scalings, use input parameter `ilhthresh` to select the scaling to use, and turn on constraint equation no. 23 with iteration variable no. 104 (`flhthresh`). By default, this will ensure that the power reaching the divertor is at least equal to the threshold power calculated for the chosen scaling, which is a necessary condition for H-mode. However, for L-mode it might be appropriate to set `boundl(104) = 0.001, boundu(104) = 1.0`, which will ensure that the power threshold does not exceed the calculated value, and therefore the machine cannot reach H-mode.

	name	reference
(1) (2) (3)	1996 ITER scaling: nominal 1996 ITER scaling: upper bound 1996 ITER scaling: lower bound	ITER Physics Design Description Document, D. Boucher, p.2-2
(4) (5)	1997 ITER scaling, excluding elongation 1997 ITER scaling, including elongation	J. A. Snipes, ITER H-mode Threshold Database Working Group, Controlled Fusion and Plasma Physics, 24th EPS Conference, Berchtesgaden, June 1997, vol.21A, part III, p.961
(6) (7) (8)	2008 Martin scaling: nominal 2008 Martin scaling: 95% upper bound 2008 Martin scaling: 95% lower bound	Martin et al, 11th IAEA Tech. Meeting on H-mode Physics and Transport Barriers, Journal of Physics: Conference Series **123** (2008) 012033

Table 3.2: *Summary of the L-H power threshold scalings implemented in `PROCESS`.*

3.1.2.14 Other plasma physics options

Neo-classical correction effects

Switch `ires` controls whether neo-classical (trapped particle) effects [30] are included in the calculation of the plasma resistance and ohmic heating power in routine `POHM`, which is called by routine `PHYSICS`. If `ires = 1`, these effects are included. Note that the scaling used is only valid for aspect ratios between 2.5 and 4, and it is possible for the plasma resistance to be wrongly calculated as negative if `ires = 1` and the aspect ratio is too high.

Inverse quadrature in τ_E scaling laws

Switch `iinvqd` determines whether the energy confinement time scaling laws (see Section 3.1.2.10) due to Kaye-Goldston (`isc = 5`) and Goldston (`isc = 9`) should include an inverse quadrature scaling with the Neo-Alcator result (`isc = 1`). A value `iinvqd = 1` includes this scaling.

Plasma / first wall gap

The region directly outside the last closed flux surface of the core plasma is known as the scrape-off layer, and contains no structural material. Plasma entering this region is not confined and is removed by the divertor. `PROCESS` treats the scrape-off layer merely as a gap. Switch `iscrp` determines whether the inboard and outboard gaps should be calculated as 10% of the plasma minor radius (`iscrp = 0`), or set equal to the input values `scrapli` and `scraplo` (`iscrp = 1`).

3.1.3 Armour, first wall and breeding blanket

The surface facing the plasma is a thin layer of a material highly resistant to melting and erosion, such as tungsten, referred to "armour". It is cooled by conduction to the first wall underneath.

The first wall sits behind the armour, and is dedicated to removing the heat landing on the armour. It does not breed tritium. Due to the hostile environment the first wall and armour have only a short lifetime and therefore need to be replaced regularly. It is cooled either by gaseous helium or by pressurised liquid water, depending on the selection of blanket type using the switch `blkttype` – see Section 3.1.3.1.

Wall load calculation

Switch `iwalld` determines whether the neutron wall load (power per unit area) should be calculated using the plasma surface area (`iwalld = 1`) or the first wall area (`iwalld = 2`) as the denominator. In the former case, input parameter `ffwal` (default value 0.92) can be used to scale the neutron power reaching the first wall.

The breeding blanket performs a number of tasks. An incoming neutron from a deuterium-tritium (D-T) fusion reaction in the plasma loses energy in the blanket. This energy is removed by the blanket coolant and used to produce electricity. The neutron may also react with a lithium nucleus present in the blanket to produce ("breed") a tritium nucleus which can be re-used as fuel. The competing requirements of heating and tritium synthesis mean that a neutron multiplier must be present, to ensure balance between tritium destruction and creation. The blanket therefore contains beryllium to fulfil this purpose. As with the first wall, the blanket has a relatively short lifetime because of the high neutron fluence.

3.1.3.1 Blanket model options

The models used for the thermoydraulics of the first wall, the profile of deposition of the neutron energy, tritium breeding, and conversion of heat to electricity have been revised extensively.

`iblanket`: This switch selects between different types of blanket.

In the CCFE HCPB (helium-cooled pebble bed) model (`iblanket = 1`), the energy deposition in the armour and first wall, blanket and shield are calculated using parametric fits to an MCNP

neutron and photon transport model of a sector of a tokamak. The blanket contains lithium orthosilicate Li_4SiO_4, titanium beryllide $TiBe_{12}$, helium and Eurofer steel.

The KIT HCPB model (`iblanket = 2`) allows the energy multiplication factor `emult`, the shielding requirements and tritium breeding ratio to be calculated self-consistently with the blanket and shielding materials and sub-assembly thicknesses, and for constraints to be applied to satisfy the engineering requirements. For further details of this model, see Section 3.1.3.2.

The CCFE HCPB model with tritium breeding ratio (`iblanket = 3`) has the features of the CCFE HCPB model above, with a set of fitting functions for calculating tritium breeding ratio (TBR). It requires a choice of `iblanket_thickness`, specifiying a THIN, MEDIUM or THICK blanket. This fixes the values of inboard and outboard blanket thickness, and the initial values of first wall thickness (3 cm) and first wall armour (3 mm). Note that these last two can be modified by the first wall thermohydraulic module, in which case the output will not be fully self-consistent. The lithium-6 enrichment and the breeder fraction (Li4SiO4/(Be12Ti+Li4SiO4) by volume) are available as iteration variables, and the minimum TBR can be set as a constraint. The maximum values of TBR achievable are as follows:
Thin: 1.247, Medium: 1.261, Thick: 1.264.

`secondary_cycle` : This switch controls how the coolant pumping power in the first wall and blanket is determined, and also how the calculation of the plant's thermal to electric conversion efficiency (the secondary cycle thermal efficiency) proceeds. See Section 3.1.12.

3.1.3.2 KIT Blanket neutronics model

The model used if `blktmodel = 1` is based on the Helium-Cooled Pebble Bed (HCPB) blanket concept developed by KIT (a second advanced model — Helium-Cooled Lithium Lead, HCLL — will be implemented in due course). The blanket, shield and vacuum vessel are segmented radially into a number of sub-assemblies. Moving in the direction away from the plasma/first wall, these are:

- Breeding Zone (BZ) (which includes the first wall), with radial thicknesses (inboard and outboard, respectively) `fwith+blbuith`, `fwoth+blbuoth`. This consists of beryllium (with fraction by volume `fblbe`), breeder material (`fblbreed`), steel (`fblss`) and helium coolant. Three forms of breeder material are available: lithium orthosilicate (Li_4SiO_4) (chosen by setting `breedmat = 1`), lithium metatitanate (Li_2TiO_3) (`breedmat = 2`) or lithium zirconate (Li_2ZrO_3) (`breedmat = 3`). The ^{6}Li enrichment percentage may be modified from the default 30% using input parameter `li6enrich`.

- Box Manifold (BM), with radial thicknesses (inboard and outboard, respectively) `blbmith`, `blbmoth` and helium fractions `fblhebmi`, `fblhebmo` (the rest being steel).

- Back Plate (BP), with radial thicknesses (inboard and outboard, respectively) `blbpith`, `blbpoth` and helium fractions `fblhebpi`, `fblhebpo` (the rest being steel).

  Together, the BZ, BM and BP make up the 'blanket', with total radial thicknesses `blnkith` (inboard) and `blnkoth` (outboard), and void (coolant) fraction `vfblkt`; Note that these quantities are *calculated* from the sub-assembly values if `blktmodel > 0`, rather than being input parameters.

- Low Temperature Shield and Vacuum Vessel (lumped together for these calculations), with radial thicknesses (inboard and outboard, respectively) `shldith+ddwi`, `shldoth+ddwi` and **water** coolant fraction `vfshld` (the rest being assumed to be steel for its mass calculation; the neutronics

model assumes that the shield contains 2% boron as a neutron absorber, but this material is not explicitly mentioned elsewhere in the code — so its cost is not calculated, for example).

N.B. The fact that water is assumed to be the coolant in the shield, whereas helium is the coolant in the blanket, leads to an inconsistency when specifying the coolant type via switch `coolwh` *(see Section 3.1.3.1). At present we mitigate this by forcing* `coolwh=2` *(making water the coolant), as in this case the coolant mass and pumping costs are higher, giving the more pessimistic solution with regards to costs.*

A few other input parameters are useful for tuning purposes, as follows:

- `fvolsi` and `fvolso` are the area (and volume) coverage factors for the inboard and outboard shields, respectively.
- `fvoldw` is a multiplier for the volume of the vacuum vessel, used in the item's mass calculation to account for ports, etc.
- `npdiv` is the number of divertor ports, used in the calculation of the tritium breeding ratio.
- `nphcdin` and `nphcdout` are the number of heating/current drive ports on the inboard and outboard sides, respectively, used in the calculation of the tritium breeding ratio. These may be either 'small' (`hcdportsize = 1`) or 'large' (`hcdportsize = 2`).
- `wallpf` is the neutron wall load peaking factor (maximum/mean), used in the calculation of the blanket lifetime.
- `ucblbreed` is the unit cost ($/kg) of the breeder material.

KIT model outputs and available constraints

The KIT blanket neutronics model provides the following outputs:

- The total nuclear power deposited in the blanket and shield, `pnucblkt` and `pnucshld`, respectively, and the energy multiplication factor in the blanket, `emult` aref calculated.
- The tritium breeding ratio, `tbr`. This can be constrained to be no less than a certain value `tbrmin` for tritium self-sufficiency by turning on constraint equation no. 52 with iteration variable no. 89 (`ftbr`). The inboard and outboard blanket BZ thicknesses, `blbuith` and `blbuoth` can also be used as iteration variables (90 and 91, respectively) to help the constraint to be met.
- The tritium production rate in grammes/day is calculated.
- The fast neutron fluence (neutrons/m^2) on the TF coils is calculated. The peak value of this quantity may be constrained to be no more than a maximum value `nflutfmax` by turning on constraint equation no. 53 with iteration variable no. 92 (`fflutf`). The inboard and outboard shield thicknesses, `shldith` and `shldoth` can also be used as iteration variables (93 and 94, respectively) to help the constraint to be met. (Note that in this calculation the TF coil case surrounding the superconductor winding pack is ignored.)
- The nuclear heating power (MW/m^3) on the inboard and outboard TF coils is calculated. Again, this can be limited to be no more than a maximum value `ptfnucmax` by turning on constraint equation no. 54 with iteration variable no. 95 (`fptfnuc`). The inboard and outboard shield thicknesses also help this constraint to be met. (Note that in this calculation the TF coil case surrounding the superconductor winding pack is ignored.) This constraint equation may also be used with `blktmodel = 0`.

- The helium concentration in the vacuum vessel at the end of the plant lifetime is calculated. This needs to be constrained for re-weldability purposes, and can be kept below a maximum value `vvhealw` by turning on constraint equation no. 55 with iteration variable no. 96 (`fvvhe`).
- The blanket lifetime is calculated, assuming a maximum allowable level of neutron damage to its steel of 60 dpa (currently not adjustable). (For the `blktmodel = 0` model, the allowable blanket fluence `abktflnc` in MW-years/m^2 may be input.)

3.1.4 Shield

The shield reduces the neutron flux reaching the vacuum vessel, TF coils and beyond. This minimises the radiological impact of the neutrons, and their heating of the TF coils which, if superconducting, need to remain at liquid helium temperatures. As with the blanket the energy deposited in the coolant may or may not be used to produce electricity, depending on the value of the switch `iprimshld` . The shield coolant fraction by volume is set via the input parameter `vfshld`.

The inboard and outboard shield thicknesses (`shldith` and `shldoth`, respectively) may be used as iteration variables.

3.1.5 Divertor

The divertor provides a means of removing plasma reaching the scrape-off layer. The principal outputs from the code are the divertor heat load, used to determine its lifetime, and its peak temperature. The divertor is cooled either by gaseous helium or by pressurised water.

Switch `snull` controls the overall plasma configuration. Setting `snull = 0` corresponds to an up-down symmetric, double null configuration, while `snull = 1` (the default) assumes a single null plasma with the divertor at the bottom of the machine. The vertical build (see Figure 3.3) and PF coil current scaling algorithms take the value of this switch into account, although not the plasma geometry at present.

The Harrison-Kukushkin-Hotston divertor model [16] developed for ITER is available, but is unlikely to be relevant for a reactor.

3.1.6 Toroidal field coils

The toroidal field (TF) coils can be either resistive or superconducting. Switch `itfsup` should be set to `1` for superconducting coils, or `0` for purely copper coils. In the superconductor model, the *CICC* (Conductor In Cable Conduit) structure shown in Figure 3.6 is assumed, and the coils are cooled using a liquid helium cryogenic system.

The steel radial plates shown in the figure help in the winding process and also provide extra support against tangential stresses. Iteration variable no. 101 (`prp`) is the ratio of the total radial plate plus steel cap cross-sectional area within the winding pack to the total winding pack cross-sectional area; from this, the half-thickness `trp` is calculated.

The outboard leg of the TF coil is assumed to be the same width in the toroidal direction as the outside edge of the inboard leg. In the radial direction, for resistive TF coils the input parameter `tfootfi` gives the ratio of the outboard leg thickness to the inboard leg thickness `tfcth`; for superconducting coils the outboard thickness is set equal to the inboard thickness.

Each TF coil is defined in the (R, Z) plane by a straight section and four elliptical arcs. Because of the finite number of TF coils used in a tokamak (18 for ITER), the toroidal field has a ripple introduced

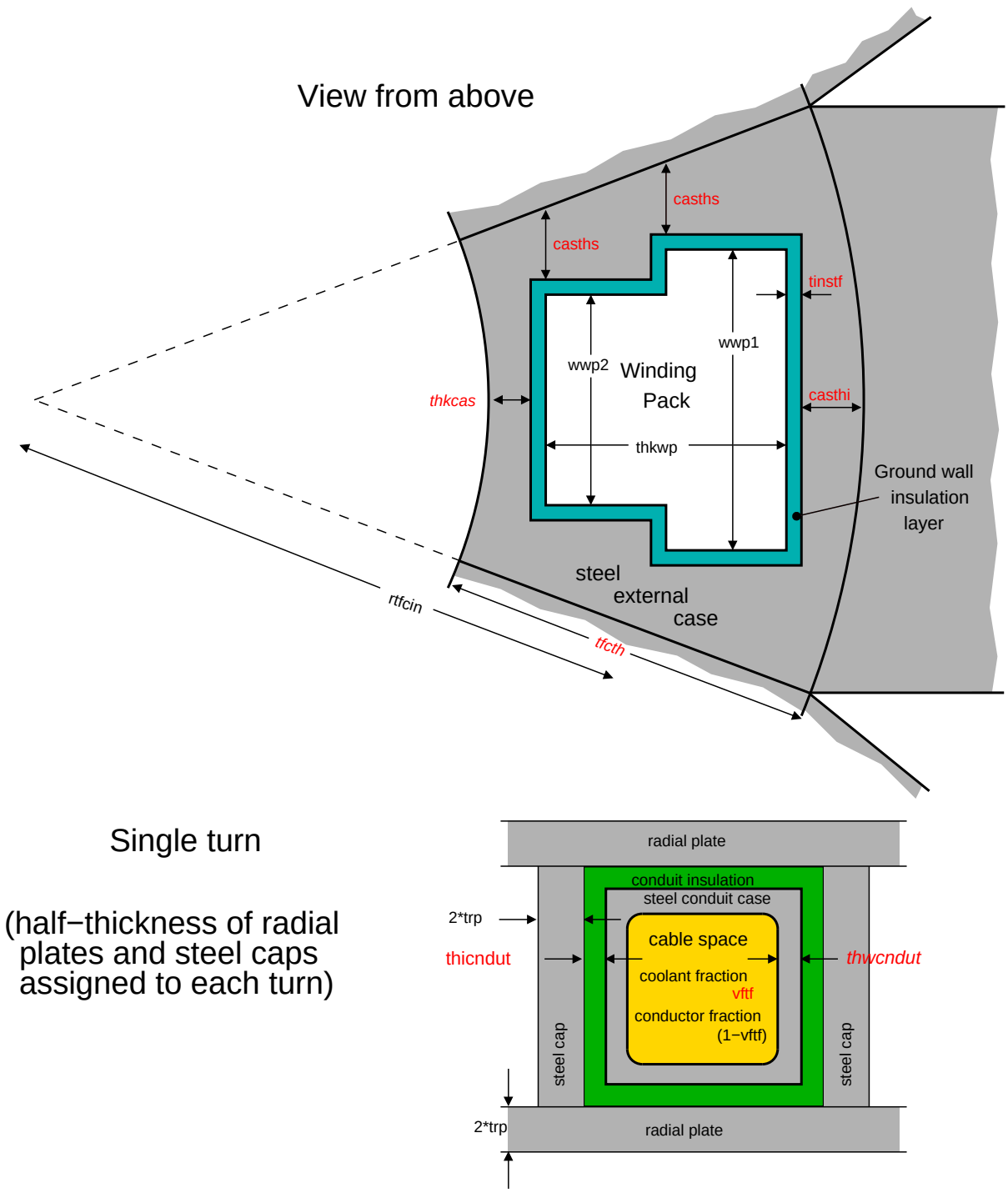


Figure 3.6: *Schematic diagram of the cross-section of the inboard leg of a superconducting TF coil, showing the CICC (Conductor In Cable Conduit) construction. The winding pack contains many turns of cable conduit. The cable space contains the superconducting filaments, and circulating liquid helium coolant. The variables shown in red may be changed by the user, and those in italics may be chosen as iteration variables.*

into it, the amplitude of which can be limited to a few percent (given by input parameter `ripmax`, default value 1%) by the code by adjusting the outboard gap thickness (labelled `gapsto` in Figures 3.1 and 3.2).

Among the TF coil parameters calculated by the code are the maximum allowable current density, the stresses on the structure, the energy stored and the magnetic field produced by the coils.

The following options are available within the superconducting TF coil model (`itfsup = 1`).

3.1.6.1 Superconducting materials

Switch `isumattf` specifies which superconducting material is to be used:

`isumattf = 1 :` Nb_3Sn superconductor, ITER critical surface parameterization [33], standard critical values

`isumattf = 2 :` Bi-2212 high temperature superconductor

`isumattf = 3 :` NbTi superconductor

`isumattf = 4 :` Nb_3Sn superconductor, ITER critical surface parameterization [33], user-defined critical parameters

The fraction of copper present in the superconducting filaments is given by the value of variable `fcutfsu` (iteration variable no. 59).

For `isumattf = 2`, a technology adjustment factor `fhts` may be used to modify the critical current density fit for the Bi-2212 superconductor, to describe the level of technology assumed (i.e. to account for stress, fatigue, radiation, AC losses, joints or manufacturing variations). The default value for `fhts` is 0.5 (a value of 1.0 would be very optimistic).

For `isumattf = 4`, important superconductor properties may be input by the user as follows: the upper critical field at zero temperature and strain is set using input parameter `bcritsc`, and the critical temperature at zero field and strain is set using input parameter `tcritsc`.

3.1.6.2 Current density limits

The current in the TF coils must be sufficient to produce the required toroidal field at the centre of the plasma. In tokamaks, the field falls off at a rate $1/R$, with the peak value occurring at the outer edge of the inboard portion of the TF coil winding pack ($R_{\text{max TF}}$ = `rbmax`). The maximum TF coil current depends on the field it produces and the allowable current density.

Three constraints are relevant to the operating current density J_{op} in the (superconducting) TF coils.

- To ensure that J_{op} does not exceed the critical value J_{crit}, constraint equation no. 33 should be turned on with iteration variable no. 50 (`fiooic`).
- To ensure that J_{op} does not exceed the current density protection limit, constraint equation no. 35 should be turned on with iteration variable no. 53 (`fjprot`).
- The critical current density J_{crit} falls with the temperature of the superconductor. The temperature margin ΔT is the difference between the temperature at which J_{crit} would be equal to J_{op} and the operating temperature. The minimum allowed ΔT can be set using input parameter `tmargmin` together with constraint equation no. 36 and iteration variable no. 54 (`ftmargtf`).

Note that if the temperature margin is positive, J_{op} is guaranteed to be lower than J_{crit}, and so constraints 33 and 36 need not both be turned on (in fact, it is recommended that only one of these two constraints is activated in any given run).

3.1.6.3 Stress model

Switch `tfc_model` controls whether a simple stress model (`tfc_model = 0`, suitable for solid copper TF coils) or a more complex stress model (`tfc_model = 1`) should be used. If `tfc_model = 1`, a two-layer stress model [35] developed by CCFE is used.

To enforce the stress limits calculated using either of these models, constraint equation no. 31 (case stress) and/or constraint equation no. 32 (conduit stress) should be turned on with iteration variables no. 48 (`fstrcase`) and/or no. 49 (`fstrcond`), respectively. The stress limit is set using input parameter `alstrtf`.

3.1.7 Poloidal field coils

The poloidal field (PF) coils are used initially to cancel the vertical field produced at the centre of the plasma by the central solenoid (Section 3.1.8) during start-up, and then to maintain the plasma position and shape during the flat-top period.

3.1.7.1 PF coil positions

The positions and sizes of the PF coils are partly input, and partly calculated after consideration of the required currents and allowable current density.

The PF coil locations are controlled using a set of switches stored in array `ipfloc` (see Figure 3.1), and are calculated in routine `PFCOIL`. The coils are (usually) organised into groups containing two PF coils placed symmetrically above and below the midplane, and each group `j` has an element `ipfloc(j)` assigned to it. Input parameter `ngrp` should be set to the number of groups, and `ncls(j)` should be assigned the number of coils in each group — which should be `2` in each case.

In the following, all variables are defined in the variable descriptor file `vardes.html`. The values for `rpf1`, `rpf2`, `zref(j)` and `routr` should be adjusted by the user to locate the PF coils accurately.

The three possible values of `ipfloc(j)` correspond to the following PF coil positions: (Redo taking into account snull and other recent changes e.g. rclsnorm)

`ipfloc(j) = 1 :` PF coils are placed above the central solenoid (one group only);

$$\begin{aligned} R &= \mathtt{rohc} + \mathtt{rpf1} \\ Z &= \pm(\mathtt{hmax} * \mathtt{ohhghf} + 0.1 + 0.5 * (\mathtt{hmax} * (1 - \mathtt{ohhghf}) + \mathtt{tfcth} + 0.1)) \end{aligned}$$

`ipfloc(j) = 2 :` PF coils are placed above the TF coils (one group only);

$$\begin{aligned} R &= \mathtt{rmajor} + \mathtt{rpf2} * \mathtt{triang} * \mathtt{rminor} \\ Z &= \pm(\mathtt{hmax} + \mathtt{tfcth} + 0.86) \end{aligned}$$

`ipfloc(j) = 3 :` PF coils are placed radially outside the TF coils (any number of groups (?));

$$\begin{aligned} R &= \mathtt{rtot} + \mathtt{tfthko}/2 + \mathtt{routr} \\ Z &= \pm(\mathtt{rminor} * \mathtt{zref(j)}) \end{aligned}$$

The void fraction (for coolant) in each coil `i`'s winding pack is given by `vf(i)`.

3.1.7.2 PF coil currents

The peak current per turn, `cptdin(i)`, and the winding pack peak current density `rjconpf(i)` in each PF coil `i` are inputs. The PF coil currents vary as a function of time during the tokamak operation as indicated in Figure 3.7. They contribute part of the flux swing necessary to maintain the plasma current (see Section 3.1.8).

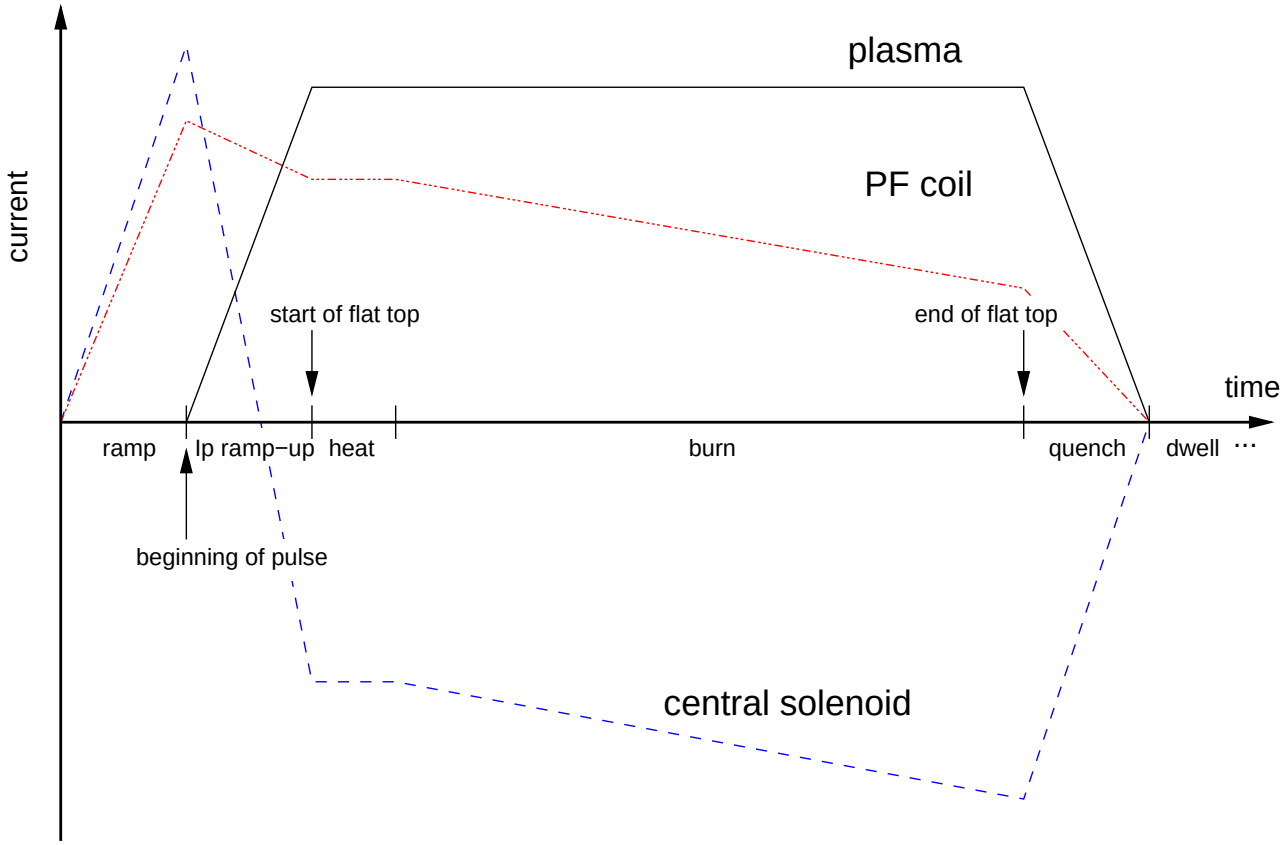


Figure 3.7: *Plot showing schematically the current waveforms for the plasma, a typical PF coil, and the central solenoid. Note that the currents in some of the PF coils may be the opposite sign to that shown, and the central solenoid current may remain positive during the I_p ramp-up period, although it will pass through zero during the burn phase.*

3.1.7.3 PF coil material

The PF coils can be either resistive or superconducting. This is determined from the value of `ipfres`. If `ipfres = 0`, the PF coils and the central solenoid are assumed to be superconducting. If `ipfres = 1`, they are assumed to be resistive, with their resistivity given by the value of variable `pfclres`.

If `ipfres = 0`, switch `isumatpf` specifies which superconducting material is to be used for the PF coils. The values for `isumatpf` are used in the same way as switch `isumattf` is for the TF coils (see Section 3.1.6.1).

The fraction of copper present in the superconducting filaments is given by the value of variable `fcupfsu`.

If the PF coils are superconducting, a steel case is assumed to surround the current-carrying winding pack to take the hoop stress. Its cross-sectional area is determined by the $J \times B$ hoop force on the

coil divided by the allowable hoop stress, given by input parameter `sigpfcalw`. The input parameter `sigpfcf` provides a scale factor (default is 0.666) to adjust the hoop force if required, to indicate what proportion of the force is supported by the case.

3.1.8 Central solenoid

Formerly known as the ohmic heating (OH) coil, the central solenoid is a PF coil used during start-up and during the burn phase to create and maintain the plasma current by inductive means. Swinging (changing) the current through the central solenoid causes a change in the flux linked to the plasma region, inducing a current in it. `PROCESS` calculates the amount of flux required to produce the plasma current, and also the amount actually available. The code measures the magnetic flux in units of Volt-seconds (= Webers).

Switch `iohcl` controls whether a central solenoid is present. A value of `1` denotes that this coil is present, and should be assigned a non-zero thickness `ohcth`. A value of `iohcl = 0` denotes that no central solenoid is present, in which case the thickness `ohcth` should be set to zero. No PF coils should be located at positions defined by `ipfloc(j) = 1` if no central solenoid is present.

The central solenoid can be either resistive or superconducting (controlled via switch `ipfres` as for the other PF coils), and if superconducting, switch `isumatoh` determines the superconducting material to use — its value is used like `isumattf` and `isumatpf`. The fraction of copper present in the superconducting filaments is given by the value of variable `fcuohsu`.

If the central solenoid is superconducting, the coil contains steel for strength. The cross-sectional area of steel is determined by the $J \times B$ hoop force on the coil divided by the allowable hoop stress, given by the input `alstroh`. A steel thickness is given in the output, which would be the thickness of a steel case of the same cross-sectional area if it simply surrounded the conducting region.

3.1.8.1 Current density inputs and limits

The (absolute value of the) central solenoid current density at the end-of-flat-top ('EOF'), `coheof` is specified by the user, and can be used as an iteration variable (no. 37). The current density at the beginning-of-pulse ('BOP' — see Figure 3.7) is specified as a (positive) fraction of `coheof` using `fcohbop` (iteration variable no. 41). The current density in the CS at all other times is calculated by taking account of the flux swing necessary to initiate and maintain the plasma current. The positive or negative sign of the current at each time is calculated automatically.

The current density in the central solenoid can be limited at the BOP and at the EOF. To limit the current density at the BOP, constraint equation no. 27 should be turned on with iteration variable no. 39 (`fjohc0`). To limit the current density at the EOF, constraint equation no. 26 should be turned on with iteration variable no. 38 (`fjohc`).

As for the TF coils, the critical current density J_{crit} falls with the temperature of the superconductor. The temperature margin ΔT is the difference between the temperature at which J_{crit}would be equal to J_{op} and the operating temperature. The minimum allowed ΔT can be set using input parameter `tmargmin` together with constraint equation no. 60 and iteration variable no. 106 (`ftmargoh`).

Note that if the temperature margin is positive, J_{op} is guaranteed to be lower than J_{crit}, and so constraints 26, 27 and 60 need not all be turned on (in fact, it is recommended that EITHER the latter constraint, OR the former two constraints, is/are activated in any given run).

3.1.8.2 Plasma current ramp-up time

In the steady-state power plant scenario (`lpulse` $\neq$ `1` — see Section 3.3), the length of time taken for the central solenoid current to (possibly) reverse (which is equal to the plasma current ramp-up time — see Figure 3.7) is determined from the value of switch `tohsin`. If `tohsin = 0`, then the plasma current ramp-up time `tohs` in seconds is given by `tohs` $= I_p/0.5$, where I_p is the plasma current in MA. Furthermore, the PF coil ramp time `tramp` and shutdown time `tqnch` are set equal to `tohs`. If `tohsin` $\neq$ `0`, the plasma current ramp-up time `tohs = tohsin`, and the PF coil ramp and shutdown times are input parameters.

If, however, a pulsed power plant is being modelled (`lpulse = 1`), the plasma current ramp-up time `tohs` is either an input parameter, or it can be iterated by using iteration variable 65. The ramp and shutdown times in the pulsed case are always set equal to `tohs`. To ensure that the plasma current ramp rate during start-up is prevented from being too high, as governed by the requirement to maintain plasma stability by ensuring that the induced current has time to diffuse into the body of the plasma, constraint equation no. 41 should be turned on with iteration variable no. 66 (`ftohs`).

3.1.9 Auxiliary power systems: heating and current drive

3.1.9.1 Current Drive

The use of inductive current drive leads to pulsed plant operation because of the limited flux swing that can be achieved using the central solenoid. This poses problems due to the fact that fatigue failures may result, and there would also be a need for thermal storage to maintain output of electricity between pulses, and supply power for starting a new pulse. However, the plasma current can also be produced and maintained (partially or wholly) using non-inductive means which, in principle, removes this restriction. `PROCESS` contains a number of auxiliary current drive schemes, including various RF methods (Lower Hybrid, Electron Cyclotron, and Ion Cyclotron (Fast Wave) current drives) and also Neutral Beam current drive systems. The code calculates the efficiency and the resulting power requirements of the chosen system.

The fraction of the required plasma current to be produced by non-inductive means, `fvsbrnni`, should be set, and flag `irfcd` should be set to `0` for purely inductive scenarios, or `1` otherwise. The current drive efficiency model to be used in this latter case is defined by the value of switch `iefrf`:-

`iefrf = 1 :` Fenstermacher Lower Hybrid model

`iefrf = 2 :` Ion cyclotron model [16]

`iefrf = 3 :` Fenstermacher electron cyclotron resonance model

`iefrf = 4 :` Ehst Lower Hybrid model

`iefrf = 5 :` ITER neutral beam model [16, 17]

`iefrf = 6 :` Culham Lower Hybrid model [17]

`iefrf = 7 :` Culham electron cyclotron model [17]

`iefrf = 8 :` Culham neutral beam model [17]

`iefrf = 9 :` Oscillating Field current drive (RFPs only — see Section 3.6.1.5)

(Note that, at present, the neutral beam models do not include the effect of an edge transport barrier (pedestal) in the plasma profile.)

It is sometimes useful to adjust artificially the current drive efficiency values produced by these routines. This can be achieved by setting the scaling coefficient `feffcd`. The wall plug to plasma efficiencies can also be adjusted, by changing the relevant variable (`etaech`, `etalh`, `etanbi` or `etaof`).

3.1.9.2 Plasma heating

In addition to current drive, some auxiliary power can be used purely to heat the plasma. The value of input parameter `pheat` determines the amount of auxiliary *heating* power (in Watts) to be applied to the plasma. This variable may be used as an iteration variable (no. 11).

3.1.9.3 Neutral beam access

If present, a neutral beam injection system needs sufficient space between the TF coils to be able to intercept the plasma tangentially. The major radius `rtanbeam` at which the centreline of the beam is tangential to the toroidal direction is user-defined using input parameter `frbeam`, which is the ratio of `rtanbeam` to the plasma major radius `rmajor`. The maximum possible tangency radius `rtanmax` is determined by the geometry of the TF coils — see Figure 3.8, and this can be enforced using constraint equation no. 20 with iteration variable no. 33 (`fportsz`). The thickness of the beam duct walls may be set using input parameter `nbshield`.

3.1.9.4 Neutral beam losses

Input parameter `forbitloss` can be used to specify the fraction of the net injected neutral beam power that is lost between the beam particles' ionisation and thermalisation (known as the first orbit loss). This quantity cannot easily be calculated as it depends on the field ripple and other three-dimensional effects. The power lost is assumed to be absorbed by the first wall.

The power in the beam atoms that are not ionised as they pass through the plasma (shine-through) is calculated by the code. There are two constraint equations that can be used to control the beam penetration and deposition, as follows:

- It is necessary to use a beam energy that simultaneously gives adequate penetration of the beam to the centre of the plasma and tolerable shine-through of the beam on the wall after the beam has traversed the plasma. The number of exponential decay lengths, τ, for the beam power to fall before it reaches the plasma centre should be in the region of $\sim$ 4–6 [17, Section 4.3.2]. Constraint equation no. 14 may be used to force τ to be equal to the value given by input parameter `tbeamin`, and is therefore in effect a beam energy consistency equation.
- Alternatively, constraint equation no. 59 with iteration variable no. 105 (`fnbshinef`) may be used to ensure that the beam power fraction emerging from the plasma is no more than the value given by input parameter `nbshinefmax`.

It is recommended that **only one** of these two constraint equations is used during a run.

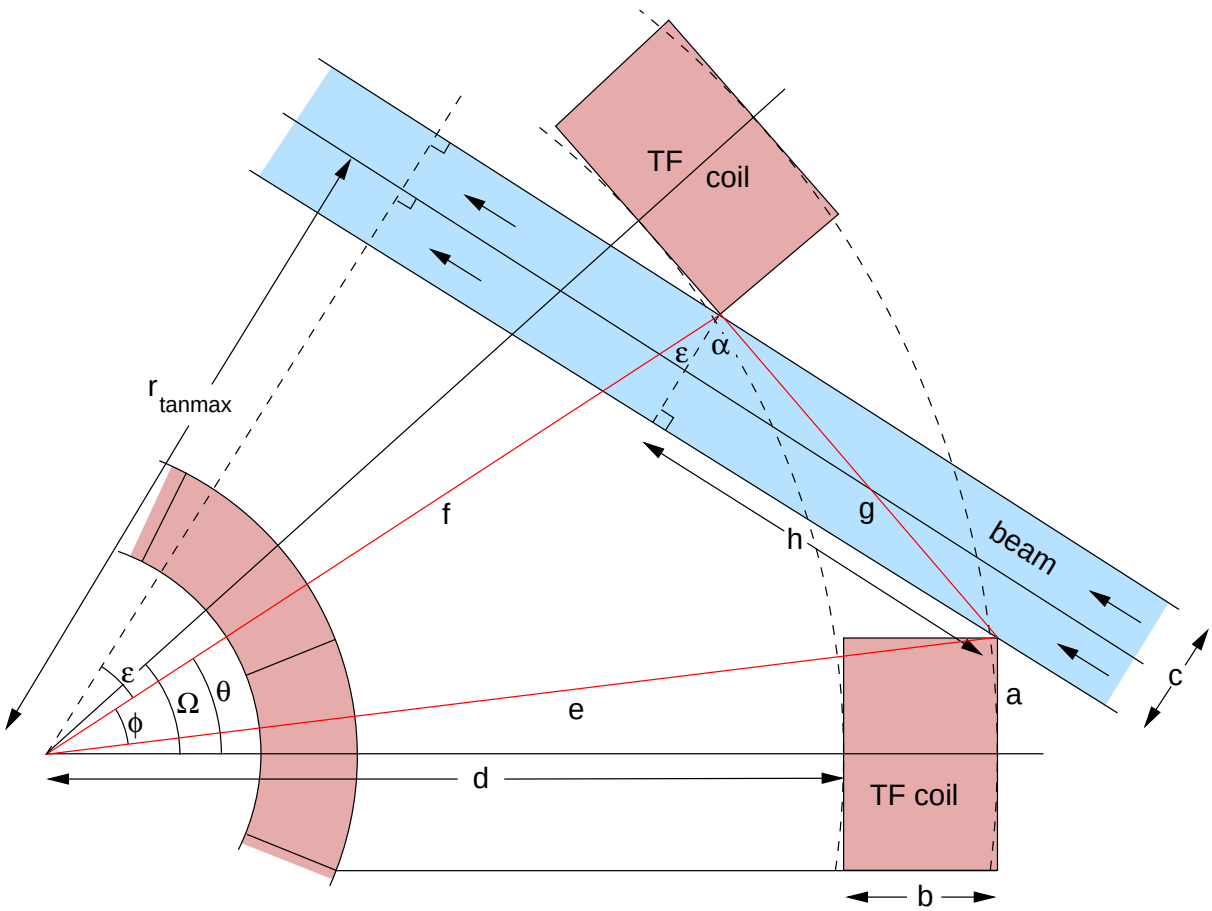


Figure 3.8: *Top-down schematic view of the neutral beam access geometry. The beam with the maximum possible tangency radius is shown here.*

3.1.9.5 Ignited plasma

Switch `ignite` can be used to denote whether the plasma is ignited, i.e. fully self-sustaining without the need for any injected auxiliary power during the burn. If `ignite = 1`, the calculated injected power does not contribute to the plasma power balance (Section 3.1.2.11), although the cost of the auxiliary power system is taken into account (the system is then assumed to be required to provide heating etc. during the plasma start-up phase only — use `pheat` to indicate the power requirement). If `ignite = 0`, the plasma is not ignited, and the auxiliary power is taken into account in the plasma power balance during the burn phase. Also, constraint equation no. 28 can be turned on to enforce the fusion gain Q to be at least `bigqmin`.

3.1.10 Structural components

Structural components are required to provide support for the fusion power core systems against gravity and the magnetic forces that will be encountered during operation. The required structural masses and their costs are calculated.

3.1.11 Cryostat and vacuum system

The internal vacuum vessel provides a toroidal evacuated chamber containing the plasma, first wall, blanket and shield, and the space between this item and the external cylindrical cryostat encloses those components that need to operate at liquid helium temperatures. These include any superconducting (TF or PF) coils and the inter-coil structure. `PROCESS` calculates the cryogenic power load and the resulting heat exchanger requirements.

The vertical distance h between the uppermost PF coil and the external cryostat lid may be adjusted by changing the value of input parameter `clhsf`; a scaling based on ITER is used:

$$h = \texttt{clhsf} \left(\frac{2 \times \texttt{rdewex}}{28.440} \right) \tag{3.22}$$

The vacuum system is used for four different processes. Firstly, before plasma operations the chamber must be evacuated to remove outgassed impurities from the structure. Secondly, the chamber must be re-evacuated between burn operations. Thirdly, helium ash must be removed to prevent it from diluting the fuel. Finally, deuterium and tritium is removed on a steady state basis. `PROCESS` calculates the parameters of a vacuum system that satisfy all four requirements, with the option of either turbo pumps or cryo pumps being used.

Switch `ntype` controls whether a turbopump (`ntype = 0`) or a cryopump (`ntype = 1`) is used in the vacuum system.

3.1.12 Power conversion and heat dissipation systems

The `PROCESS` power plant takes into account all the systems required to perform the necessary conversion of fusion power to electricity, from the coolant systems in the plant components to the heat exchangers and turbines.

Figure 3.9 shows the overall power transfer mechanisms within the power plant outside of the plasma. The efficiency of the primary coolant pumps in converting electrical to mechanical power is given by input parameter `etahtp` in all the calculations described below.

3.1.12.1 Divertor

All of the charged particle transport power leaving the plasma (excluding the `1-falpha` portion of the alpha power that escapes directly to the first wall — Section 3.1.2.11) is assumed to be absorbed in the divertor, along with a proportion `fdiv` of the radiation power and the neutron power.

Switch `iprimdiv` may be used to specify whether the thermal power deposited in the divertor becomes high-grade thermal power (`iprimdiv = 1`) or low-grade waste heat (see Figure 3.9).

3.1.12.2 First wall

The remaining photon power (i.e. the fraction not incident upon the divertor or lost through holes or the heating / current drive apparatus) is assumed to be absorbed by the first wall. Power due to ions derived from the neutral beams but lost before being thermalised (known as "first orbit loss"), and from the fast alpha particles lost before being thermalised, also contribute to the total thermal power absorbed by the first wall.

3.1.12.3 Power conversion cycle

Figure 3.9 summarises the power conversion mechanisms.

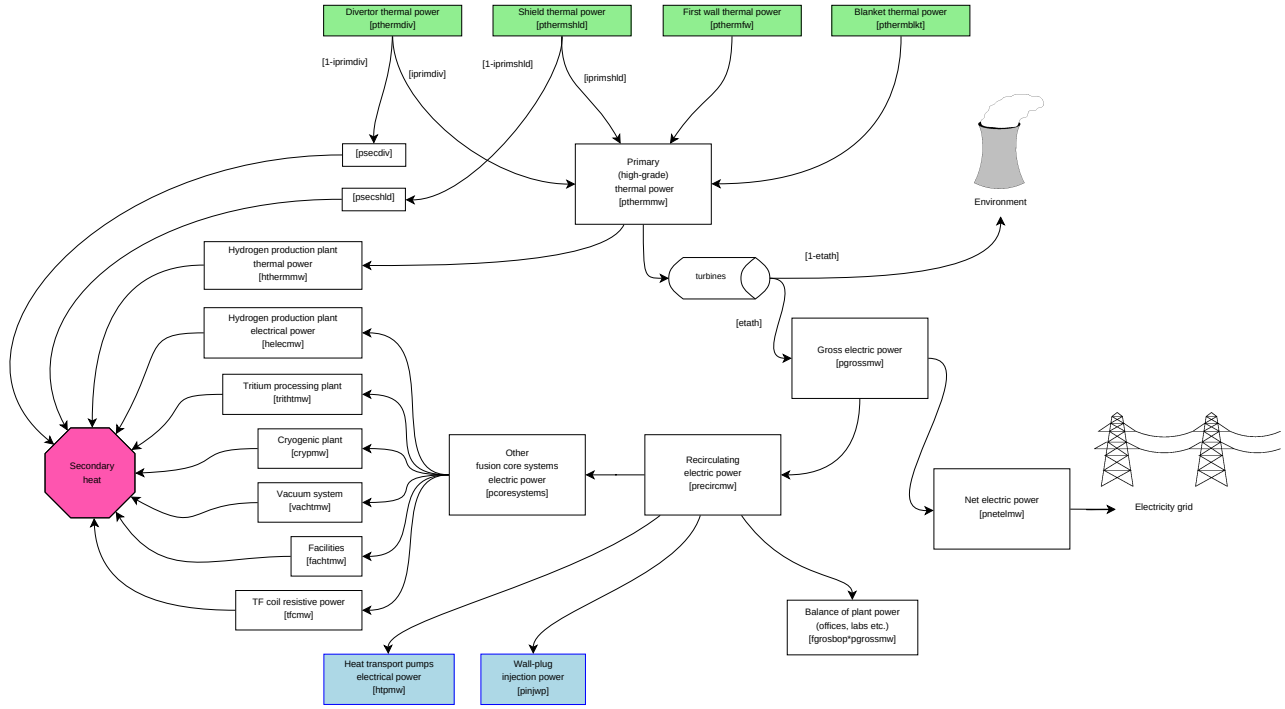


Figure 3.9: *Schematic diagram of the flow of power beyond the fusion power core, showing the origin of the high-grade and waste heat and the electrical power balance within the plant. Variable names are given in [...]. The input power contributions in green boxes originate in Figure* **??**.

The high-grade, i.e. useable thermal power (less any thermal power required to produce hydrogen in a hydrogen production plant — see Section 3.4) is used to produce steam to turn the turbines, thus generating the plant's gross electrical power, with an efficiency given by quantity `etath`. The remainder is dumped to the environment through the condenser. All of the low-grade heat is dumped to the environment.

`primary_pumping` : This switch controls the calculation of the mechanical pumping power required for the primary coolant.

If `primary_pumping = 0`, the user sets mechanical pumping power directly.

If `primary_pumping = 1`, the user sets mechanical pumping power as a fraction of thermal power removed by coolant.

If `primary_pumping = 1`, the mechanical pumping power is calculated, as follows.

User inputs for the coolant outlet temperature (which may be used as an iteration variable), the coolant channel diameter, and the segmentation of the blanket are used. The peak temperature in the first wall material (underneath the armour) is derived. The user can apply an upper limit to this temperature, and if this constraint is used then it is strongly recommended to set the length of a first wall pipe (`fw_channel_length`)as an iteration variable. The Gnielinski correlation is used to determine the heat transfer in the channel. The stresses in the first wall are not currently taken into account.

The mechanical pumping power required for the first wall and breeder zone is calculated using the Darcy friction factor, estimated from the Haaland equation, an approximation to the ColebrookWhite equation. (If you consider that the calculated value for the pumping power is too low, then you can add an additional electric power requirement using `baseel`. Do not use `htpmw_min` as this prevents the optimisation of the first wall.) The inlet and outlet temperatures of the first wall and blanket can be different. The isentropic efficiency of the first wall and blanket coolant pumps (enthalpy increase in the fluid for isentropic compression divided by the mechanical power used) is specified by the parameter `etaiso`. Note that the mechanical pumping powers for the shield and divertor are still calculated using the simplified method (a fixed fraction of the heat transported).

`secondary_cycle` : This switch controls how the calculation of the plant's thermal to electric conversion efficiency (the secondary cycle thermal efficiency) proceeds. See also Section 3.1.12, which describes the flow of power through the fusion power core.

If `secondary_cycle = 0`, the efficiency of the power generation cycle is set to a single value obtained from previous cycle modelling studies. The heat deposited in theToroidal field coils divertor coolant is assumed to be at such low temperature that it cannot be used for power generation and is dumped to the environment.

If `secondary_cycle = 1`, the efficiency of the power generation cycle is set as above, but the divertor heat is used for electricity generation.

In the remaining options (`secondary_cycle = 1, 2 or 3`), the heat deposited in the divertor coolant is used for power generation.

If `secondary_cycle = 2`, the efficiency of the power generation cycle is input by the user.

If `secondary_cycle = 3`, a steam Rankine cycle is assumed. The secondary cycle thermal efficiency (`etath`) is calculated from the coolant outlet temperature using simple relations between temperature and efficiency [32]:

$$\eta = -2.0219 + 0.3720 \ln(T) \quad \text{(water coolant; saturated steam Rankine cycle)} \tag{3.23}$$

$$\eta = -0.8002 + 0.1802 \ln(T) \quad \text{(helium coolant; superheated steam Rankine cycle)} \tag{3.24}$$

If `secondary_cycle = 4`, a supercritical CO_2 Brayton cycle is assumed. The secondary cycle thermal efficiency (`etath`) is calculated from the coolant outlet temperature using simple relations between temperature and efficiency from [32]:

$$\eta = -2.5043 + 0.4347 \log(T) \quad \text{(water or helium coolant} \tag{3.25}$$

In the above three equations, T is the temperature of the (secondary) coolant at the inlet to the turbine, assumed to be a fixed margin below the outlet temperature of the primary coolant.

The electrical power required to operate the power plant itself is the so-called recirculating electric power. Any surplus is exported to the electricity grid as net electric power.

The recirculating power comprises the electrical power required to run all of the associated electrical systems surrounding the fusion power core, plus the on-site building services, offices, etc., as shown in Figure 3.9. Of these, the cryogenic plant power includes the power required to cool the TF coils from the neutron power absorbed by the coils, the PF coils (as defined by the ratio of the total PF coil stored energy to the fusion power pulse time `tpulse`), and other 'cold' components.

3.1.13 Buildings

The volume and ground area of all the various buildings on a power plant site are included in the `PROCESS` calculations for the benefit of the costing algorithms.

3.2 Spherical Tokamak Model

`PROCESS` has the ability to perform studies on tokamaks in the low aspect ratio regime (major radius $\leq 2\times$ minor radius). The physics and engineering issues [37] associated with these machines are somewhat different from those of conventional aspect ratio, and this is reflected by the following special models [2] in `PROCESS`.

1. The inboard build of a spherical tokamak (ST) is very different from that in a conventional tokamak. There is no inboard blanket (and possibly no inboard shield), and the inboard TF coil legs are replaced by a single centrepost. The radial build is altered so that, starting from the centreline ($R = 0$), the component order is: TF coil, gap, central solenoid, vacuum vessel, and then continuing as in Figure 3.1 (a D-shaped cross-section is assumed for the first wall, blanket, shield and vacuum vessel).

2. Spherical tokamaks have resistive TF coils that combine into a single centrepost at the centre of the machine. The centrepost is constructed from copper (as are the outboard TF coil sections), and is tapered lengthways so that it is narrowest at the midplane of the device. Routine `CNTRPST` calculates various parameters relevant to the centrepost, including the pump pressure, maximum temperature and pipe radius, and these may be limited using constraint equations 43 to 46 if required:

   - Equation 43 is a consistency equation for the average centrepost temperature.
   - Equation 44 can be used to limit the peak centrepost temperature to a maximum value (`ptempalw`) using iteration variable no. 68 (`fptemp`).
   - Equation 45 can be used to force a lower limit to the edge safety factor q_{lim} (see below), using iteration variable no. 71 (`fq`).
   - Equation 46 can be used to apply an upper limit to the ratio of plasma current to TF coil ("rod") current, using iteration variable no. 72 (`fipir`).

3. A gaseous divertor model is used, and a simple divertor heat load calculation is employed, rather than the more complex divertor model assumed for conventional aspect ratio tokamaks.

4. A simple PF coil current scaling algorithm is available for use with the ST option.

5. The plasma shaping terms (elongation and triangularity) can be calculated directly given the aspect ratio, using `ishape = 1` (see Section 3.1.2.1). This setting also scales the lower limit [2] for the edge safety factor, for use with constraint equation no. 45:

$$q_{lim} = 3\,(1 + 2.6 * \epsilon^{2.8}) \tag{3.26}$$

   where $\epsilon = a/R$.

6. Among the physics models that differ from those relevant to conventional aspect ratio machines are (i) the plasma poloidal field B_{pol}, (ii) the bootstrap current fraction, (iii) the beta limit, and (iv) the neutron heating of the centrepost [2].

3.2.1 Spherical tokamak switches

Switch `itart` provides overall control of the ST switches within the code, and subroutine `CHECK` ensures that no conflicting values are inadvertently set by the user in the input file. Table 3.3 summarises the switch values relevant to each aspect ratio regime.

switch	conventional aspect ratio `itart = 0`	low aspect ratio `itart = 1`
`ishape` (Section 3.1.2.1)	0, 2	0, 1
`ibss` (Section 3.1.2.12)	1, 2, 3	2, 3
`icurr` (Section 3.1.2.8)	1, 3, 4, 5, 6, 7	2
`itfsup` (Section 3.1.6)	0, 1	0

Table 3.3: *Summary of the switch values in PROCESS that relate to conventional aspect ratio and low aspect ratio machines.*

3.3 Pulsed Plant Operation

If the plasma current is partially or entirely driven by electromagnetic induction, it is necessary to operate the plant in a pulsed manner as the current swing in the central solenoid coils cannot be continued indefinitely. `PROCESS` can perform a number of calculations relevant to a pulsed power plant, as detailed below.

Switch `lpulse` determines whether the power plant is assumed to be based on steady-state (`lpulse = 0`) or pulsed (`lpulse = 1`) operation.

3.3.1 Thermal cycling package

Update... This performs calculations on the first wall of the machine. Evaluation of the mechanical and thermal stresses on this component lead to a measure of the maximum number of cycles to which the first wall can be subjected, and hence to the minimum allowable length of each reactor cycle for a specified first wall lifetime. The cycle time can be constrained to be at least the minimum value by turning on constraint equation no. 42 with iteration variable no. 67 (`ftcycl`).

The thickness of the first wall is constrained to lie within lower and upper bounds, which ensures that it can withstand the internal coolant pressure and the peak temperature and neutron fluence.

Switch `itcycl` activates the desired model for the first wall axial stress calculations. If `itcycl = 1` (the default), the wall is fully constrained axially, and no bending can occur. If `itcycl = 2`, there is no constraint on the axial motion, but no bending can occur. Finally, if `itcycl = 3`, again there is no axial constraint, and bending is allowed to occur.

3.3.2 First wall coolant temperature rise limit

The rise in temperature of the first wall coolant can be limited to be no more than the value of `dtmpmx` by turning on constraint equation no. 38 with iteration variable no. 62 (`fdtmp`).

3.3.3 First wall peak temperature limit

The maximum first wall temperature can be limited to be no more than the value of variable `tpkmax` by turning on constraint equation no. 39 with iteration variable no. 63 (`ftpeak`).

3.3.4 Start-up power requirements

The minimum auxiliary power required during the start-up (ignition) phase is calculated on the basis of a POPCON analysis. Ignition is accessed via the so-called Cordey Pass (the path in plasma density–temperature space which minimises the power requirement) and the code ensures that there is sufficient auxiliary power to accommodate this. In fact, this calculation is very CPU-intensive, so the relevant routine is not called at present. In practice, the auxiliary power tends to exceed the minimum allowable value anyway, without any need to constrain it to do so.

The auxiliary power reaching the plasma can be forced to be more than the minimum allowable value `auxmin` by turning on constraint equation no. 40 with iteration variable no. 64 (`fauxmn`). The value of `auxmin` is determined by the code if the start-up model is activated, otherwise it may be initialised via the input file.

3.3.5 Plasma current ramp-up time

This calculation ensures that the plasma current ramp rate during start-up is prevented from being too high, as governed by the requirement to maintain plasma stability in l_i - q_ψ space (see Section 3.1.8.2).

3.3.6 Burn time

The length of the burn time is calculated from the surplus volt-seconds available from the OH/PF coil system during the plasma burn phase, after the flux required during the plasma start-up is taken into account. A minimum burn time can be enforced via constraint equation no. 13 and iteration variable no. 21 (`ftburn`).

3.3.7 Thermal storage

During every cycle there is a period when no fusion power is produced. The net electric output from the plant must, however, be maintained, and this is achieved using thermal storage. There are three types of thermal storage available within `PROCESS`, and the value of switch `istore` determines which is to be used. If `istore = 1` (the default), option 1 of Ref. [38] is assumed, which utilises the thermal storage inherent in the machine's steam cycle equipment. This should be used if the machine down

time is less than 100 seconds. If `istore = 2`, option 2 of Ref. [38] is assumed, which uses the same method as before, but augments it with an additional boiler. This may be used for machine down times of up to 300 seconds. Finally, if `istore = 3`, a large stainless steel block acts as the thermal storage medium.

3.4 Hydrogen Production Facility

Fusion power plants have been mooted as a means of producing hydrogen for use in fuel cells for cars, for instance. `PROCESS` includes options to enable the plant to produce hydrogen using a number of different processes.

To include the production of hydrogen by the power plant, it is necessary to set the switch `ihplant`, as follows:

`ihplant = 0 :` No hydrogen production (default)

`ihplant = 1 :` Hydrogen production by low temperature electrolysis

`ihplant = 2 :` Hydrogen production by endothermic high temperature electrolysis

`ihplant = 3 :` Hydrogen production by exothermic high temperature electrolysis

`ihplant = 4 :` Hydrogen production by thermo-chemical processes

Table 3.4 describes the additional options available for each of the types of hydrogen production given above. The different processes use either electrical power or thermal power directly, so the required inputs differ. Variable `helecmw` (iteration variable no. 87) is the electrical power in MW required for hydrogen production, while `hthermmw` (iteration variable no. 88) is the thermal power required. Note that `hthermmw` must not be used as an iteration variable if `ihplant` $\neq$ `4`, as it will be calculated from the required electrical power instead. Similarly, `helecmw` must not be used as an iteration variable if `ihplant = 4`.

hydrogen plant option	`helecmw`	`hthermmw`	efficiency variable
`ihplant=1`	input	zero	`etahlte`
`ihplant=2`	input	calculated	`etahten`
`ihplant=3`	input	calculated	`etahtex`
`ihplant=4`	zero	input	`etahth`

Table 3.4: *Summary of the variables in PROCESS that relate to the different hydrogen plant processes.*

The efficiency variables given in Table 3.4 are all input parameters, and are the factors to be used to convert the value of `helecmw` to the amount of hydrogen produced (in MW equivalent); these can be greater than unity in all cases except `ihplant = 4`.

3.5 Stellarator Model

The code has the ability to perform calculations based on the physics and engineering of a stellarator, which, although being a toroidal device, is radically different in a number of ways from a tokamak.

The model is largely based on W7-X and the HELIAS 5-B stellarator power plant design [39] (Figure 3.10) and related modelling that has been performed by IPP Greifswald [40, 41, 42].

To activate the stellarator coding, it is necessary to create a file `device.dat`, containing the single character `1` in the first row, in the working directory (see Section 4.4). This has the effect of setting the internally-used switch `istell = 1`. If the file is absent, or its first character is set to something other than `1`, the stellarator model is not used, and `istell` is set to `0`.

The stellarator model is largely contained within source file `stellarator.f90`. The following consistency equations (see Section 2.5) should be used without modification:

`1 :` plasma beta consistency

`2 :` global power balance

`11 :` radial build consistency

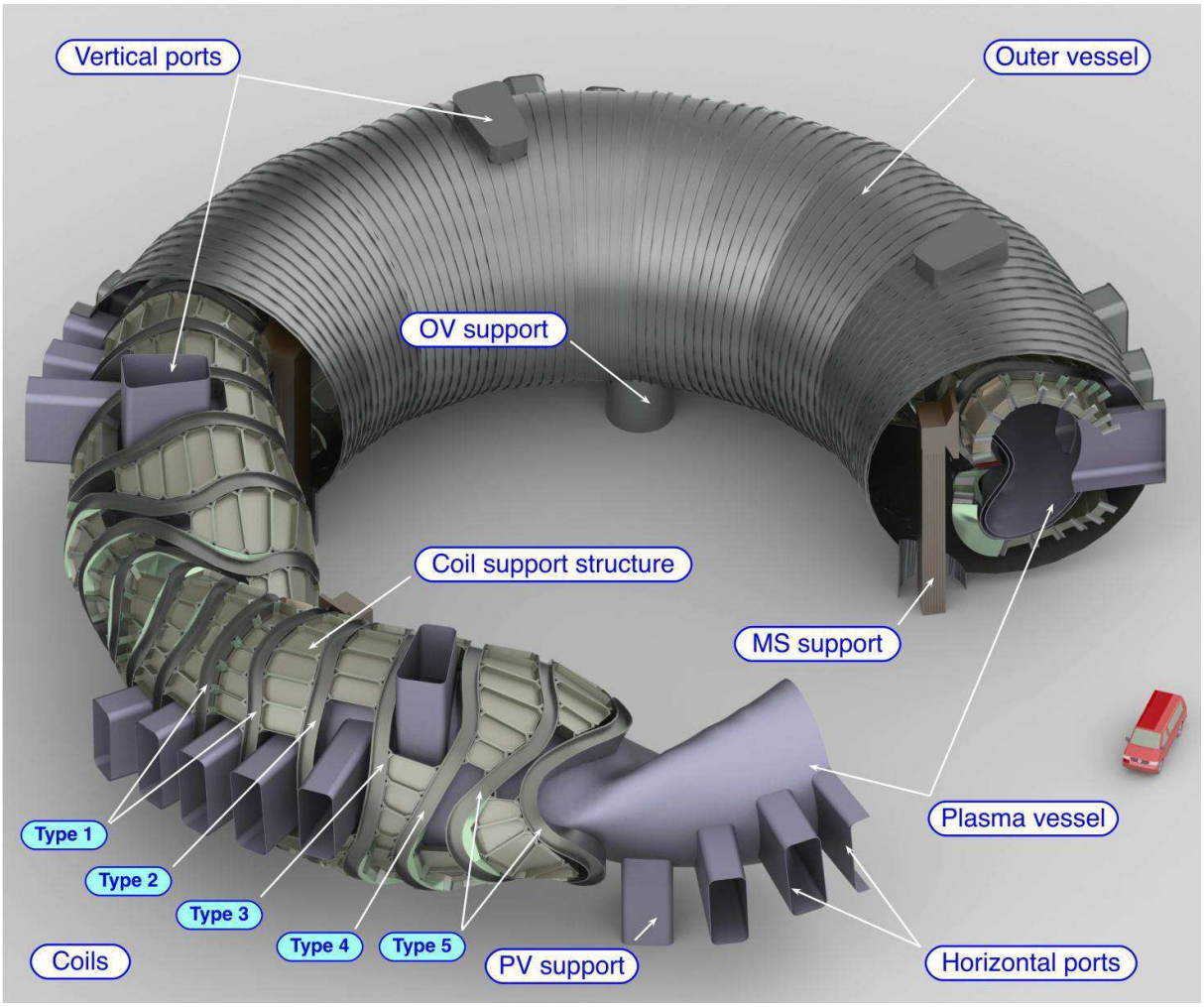


Figure 3.10: *Fusion power core of the HELIAS 5-B conceptual power plant design (from [39])*

3.5.1 Stellarator physics

Much of the physics is identical to that for tokamaks, including the plasma composition and the fusion power calculations. However, some physics topics do differ between stellarators and tokamaks, as follows.

3.5.1.1 Plasma geometry

The plasma geometry model uses Fourier coefficients to represent the complex 3-D plasma shape typical of stellarators. A VMEC [43] calculation (or other equilibrium code that can provide the Fourier coefficients of the LCFS) must have been performed prior to running with `PROCESS`. The overall size of the plasma is scaled correctly for the required (mean) major and minor radii for the machine being modelled [44].

It is necessary to provide three input files that define the plasma shape:

1. Set `vmec_info_file` in the input file to the name of a file with the following format (the numbers given are those for the W7-X high mirror configuration); in practice only the effective major and minor radius values (`R_eff` and `a_eff`, respectively) and the number of field periods are used:

```
R_eff [m]   a_eff [m]   Aspect ratio   Plasma vol [m3]  LCFS surf area [m2]  field periods
5.486576    0.4942638   11.10050       26.45749         133.4281             5.0
```

2. Set `vmec_rmn_file` in the input file to the name of a VMEC output file containing the calculated plasma boundary $R(m, n)$ Fourier coefficients, where $m = 0$ to 11 (rows) and $n = -12$ to 12 (columns).

3. Set `vmec_zmn_file` in the input file to the name of a VMEC output file containing the calculated plasma boundary $Z(m, n)$ Fourier coefficients, where $m = 0$ to 11 (rows) and $n = -12$ to 12 (columns).

This method enables a wide range of potential plasma geometries to be modelled, if required. The plasma volume, surface area and mean cross-sectional area are the outputs from the plasma geometry model.

3.5.1.2 Absense of plasma current

Stellarators try to achieve zero plasma current in order to allow safe divertor operation, so no current scalings are required.

3.5.1.3 Beta limit

The beta limit is assumed to be 5%, based on 3-D MHD calculations [45]. To apply the beta limit, constraint equation no. 24 should be turned on with iteration variable no. 36 (`fbetatry`).

3.5.1.4 Density limit

The density limit relevant to stellarators has been proposed to be [46]

$$n_{\max} = 0.25 \left(P B_0 / R_0 \, a_p^2 \right)^{\frac{1}{2}} \tag{3.27}$$

where n is the line-averaged electron density in units of 10^{20} m^{-3}, P is the absorbed heating power (MW), B_0 is the on-axis field (T), R_0 is the major radius (m), and a_p is the plasma minor radius (m). To enforce the density limit, turn on constraint equation no. 5 with iteration variable no. 9 (`fdene`).

3.5.1.5 τ_E scaling laws

Five confinement time scaling laws relevant to stellarators are present within PROCESS. The value of switch isc determines which of these is used in the plasma energy balance calculation.

$$\tau_E \text{ (Large Helical Device [46]: } \texttt{isc=21}) = 0.17\, R_0^{0.75}\, a_p^2\, \bar{n}_{20}^{0.69}\, B_0^{0.84}\, P^{-0.58} \tag{3.28}$$

$$\tau_E \text{ (Gyro-reduced Bohm [47]: } \texttt{isc=22}) = 0.25\, B_0^{0.8}\, \bar{n}_{20}^{0.6}\, P^{-0.6}\, a_p^{2.4}\, R_0^{0.6} \tag{3.29}$$

$$\tau_E \text{ (Lackner-Gottardi [48]: } \texttt{isc=23}) = 0.17\, R_0\, a_p^2\, \bar{n}_{20}^{0.6}\, B_0^{0.8}\, P^{-0.6}\, \iota^{0.4} \tag{3.30}$$

$$\tau_E \text{ (ISS95 [49]: } \texttt{isc=37}) = 0.079\, R_0^{0.65}\, a_p^{2.21}\, \bar{n}_{19}^{0.51}\, B_0^{0.83}\, P^{-0.59}\, \bar{\iota}^{0.4} \tag{3.31}$$

$$\tau_E \text{ (ISS04 [50]: } \texttt{isc=38}) = 0.134\, R_0^{0.64}\, a_p^{2.28}\, \bar{n}_{19}^{0.54}\, B_0^{0.84}\, P^{-0.61}\, \bar{\iota}^{0.41} \tag{3.32}$$

Here, $\bar{\iota}$ is the rotational transform, which is equivalent to the reciprocal of the tokamak safety factor q.

3.5.1.6 Heating power options

Stellarators require no current drive, although provision for auxiliary heating does need to be present. The method by which auxiliary heating power is supplied is determined by the switch isthtr:

isthtr = 1 : electron cyclotron resonance heating

isthtr = 2 : lower hybrid heating

isthtr = 3 : neutral beam injection

The value of variable pheat determines the actual amount of auxiliary heating power (in Watts) to be applied to the plasma. This variable may be used as an iteration variable (no. 11). Switch ignite may be used if necessary — see Section 3.1.9.5.

3.5.1.7 Divertor

Although the divertor has the same function in both stellarators and tokamaks, the envisaged concepts differ quite substantially. This is not only related to the different geometry and symmetries but also specifically to the magnetic configuration. While the inherent axisymmetry of a tokamak allows for poloidally-continuous single or double divertor configurations, the periodicity of helical advanced stellarators leads to multiple X-points with a corresponding chain of magnetic islands. This island structure may be exploited by carefully placing divertor plates along the stochastic field lines, naturally leading to a discontinuous divertor, with the individual plates being placed in a complex 3-D geometry; see Figure 3.11.

Rather than trying to describe the complex physics with a two-point scrape-off layer model as is used for tokamaks, the stellarator divertor model [41] is based on fundamental principles which relate the power crossing the separatrix with an effective wetted area on the divertor plates allowing the code to estimate the heat load delivered to the divertor. A basic island divertor model is used which assumes diffusive cross-field transport and high radiation at the X-point,

The radiated power fraction in the scrape-off layer is given by the input parameter f_rad. This is in contrast to the method used for tokamaks, in which the radiated power fraction is a calculated quantity.

A number of other input parameters may be used to modify the divertor model; see the variable descriptor file for more details.

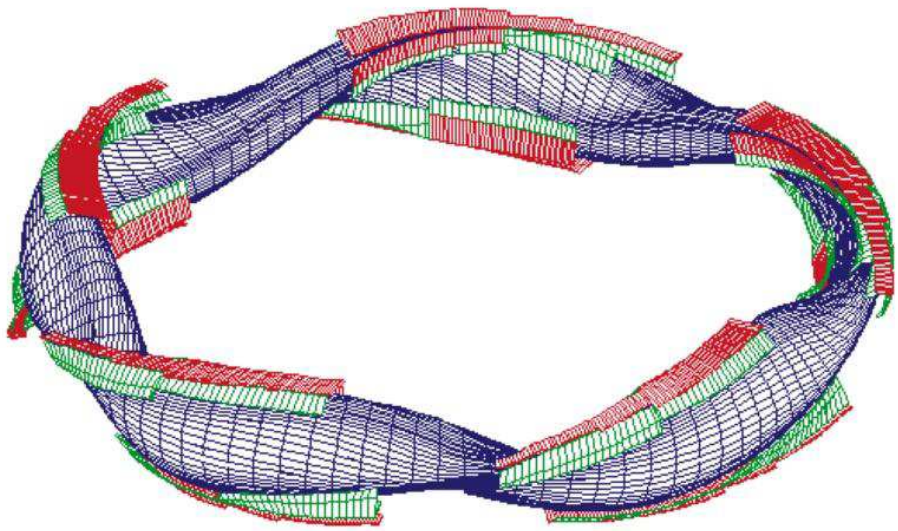


Figure 3.11: *A five-period HELIAS plasma (specifically W7-X) with island divertor plates shown in red*

3.5.2 Machine configuration

There are a large number of possible stellarator configurations. As stated earlier, the one chosen for the `PROCESS` model is based on the **HELI**cal **A**dvanced **S**tellarator (HELIAS) concept, in which all the coils resemble distorted, non-planar TF coils — no helical coils or tokamak-like PF coils are present. The coil geometry is scaled from the HELIAS 5-B power plant design, which is based on a five field-period HELIAS configuration.

3.5.2.1 Machine build

Since a stellarator is inherently non-axisymmetric, the build of the `PROCESS` stellarator is defined in terms of the mean thicknesses of components.

The surface areas for the first wall, blanket and shield components are scaled linearly with their effective minor radius from the plasma surface area calculation (the area of a simple torus of circular cross-section is $4\pi^2 Ra$, hence the linear scaling with a). The input parameter `fhole` may be used to specify the hole fraction, to adjust the surface area to take account of ports and divertors, for instance. The volumes of the first wall etc. are simply given by the product of their surface area and their mean thickness.

In contrast to tokamaks, which in `PROCESS` are assumed to have a cylindrical external cryostat completely surrounding the fusion power core, the stellarator model assumes that the external cryostat (labelled as the outer vessel in Figure 3.10) is toroidal with a circular cross-section. Its cross-section is assumed to be centred at the mean plasma major radius.

All items external to the fusion power core (buildings, turbines, power conversion systems, etc.) remain unchanged.

3.5.2.2 Stellarator coils

The stellarator coil model [42, 51] combines scaling aspects based on the HELIAS 5-B design in combination with analytic inductance and field calculations.

The fully three-dimensional shape of the coils is assumed to be fixed, but the sizes of the coils are scaled from the HELIAS 5-B values to the geometrical values for the machine being modelled using fundamental physics and engineering principles.

The stellarator coils are assumed to be superconducting — no resistive coil calculations are performed. The critical field at the superconductor is calculated using circular approximations for the coils in the inductance and field calculations, and the limit is enforced automatically. Available superconductors are Nb_3Sn (`isumattf = 1`) and NbTi (`isumattf = 3`).

The winding pack cross-section is rectangular for the stellarator coils, rather than the complicated two-step cross-section assumed for tokamaks. The coil thicknesses and most of the dimensions of the materials within the coil cross-section are outputs from the model, instead of being inputs as is the case for tokamaks; see the variable descriptor file for details. In addition, certain iteration variables (`tfcth`, no. 13; `thkcas`, no. 57; `cpttf`, no. 60 and `tftort`, no. 77) should not be turned on in the input file as they are calculated self-consistently; the code will stop with an error message if this is attempted.

3.6 Reversed Field Pinch Model

In addition to the tokamak and stellarator magnetic confinement devices, the code has the ability to perform calculations based on the physics and engineering of a reversed field pinch (RFP) device. This third type of toroidal magnetic device is superficially similar in design to a tokamak (so therefore shares many of the same components), but the magnetic field configuration differs.

The model used in `PROCESS` is largely based on the TITAN fusion power plant [52, 53]. The following sections summarise its main features, where they differ from those for tokamaks.

To activate the RFP coding, it is necessary to create a file `device.dat`, containing the single character `2` in the first row, in the working directory (see Section 4.4). This has the effect of setting the internally-used switch `irfp = 1`. If the file is absent, or its first character is set to something other than `2`, the RFP model is not used, and `irfp` is set to `0`.

3.6.1 RFP physics

The plasma in RFPs is circular in cross-section and is axisymmetric.

3.6.1.1 Beta limit

The poloidal beta is limited to a maximum value given by input parameter `betpmx` (default = 0.19) using constraint equation 48 and iteration variable 79 (`fbetap`).

3.6.1.2 Density limit

No density limit is explicitly coded for RFPs, other than by simply constraining the upper bound of the electron density variable `dene` (iteration variable 6).

3.6.1.3 τ_E scaling law

One confinement time scaling law relevant to RFPs is present within `PROCESS`. The value of switch `isc` determines the scaling to be used in the plasma energy balance calculation.

$$\tau_E \text{ (TITAN RFP [52]: } \texttt{isc=25}) = 0.05\, a^2\, I_p(\text{MA})$$

3.6.1.4 F-Θ plot

Much of the RFP physics is derived from the characteristic F-Θ plot, where $F = B_\phi(a)/\langle B_\phi \rangle$, $\Theta = B_\theta(a)/\langle B_\phi \rangle$, and $\langle B_\phi \rangle$ is the average value of the toroidal field over the plasma cross-section. Given a value of the pinch parameter Θ, the corresponding value of the reversal parameter F may be read from the F-Θ plot, and from these the plasma current and the current in the TF coils may be obtained using

$$\begin{aligned} B_\theta(a) &= \frac{\mu_0 I_p}{2\pi a} \\ B_\phi(a) &= \frac{\mu_0 I_{TFC}}{2\pi R} \end{aligned}$$

(the second of these assumes that $B_\phi(a)$ is approximately equal to the vacuum toroidal field at the plasma centre).

The pinch parameter Θ is set using iteration variable no. 78: `rfpth`. The corresponding value of the reversal parameter F (`rfpf`) is calculated using routine `FTHETA`. F is constrained to be negative using constraint equation no. 49 with f-value `frfpf` (iteration variable no. 80).

3.6.1.5 Current drive

The RFP oscillating field current drive option is turned on by setting `iefrf = 9`, with a fixed efficiency of 0.8 Amps per Watt of power injected into the plasma (the coding for this model is, therefore, trivial). The wall plug to injector efficiency is set using input parameter `etaof`, which has a default value of 0.5, and the unit cost is set using input parameter `ucof`. The default value for `ucof` is 3.3 $ per Watt of injected power.

The bootstrap fraction is assumed to be zero.

Plasma ignition, and additional plasma heating using auxiliary power, are treated as for tokamaks.

3.6.2 TF coils

The TF coils for the RFP option are derived from the TITAN-II coil set, which uses circular copper coils. The radial thickness is set using `tfcth` as usual, but the toroidal thickness may also be set, using iteration variable no. 77 (`tftort`). This is constrained to be no larger than is geometrically possible using constraint equation no. 47 with iteration variable no. 76 (`frfptf`).

3.6.3 Ohmic heating coils

The TITAN-I ohmic heating coil locations, currents etc. are assumed. These comprise 14 copper coils, with currents swinging from positive to negative during the plasma start-up period, and then decaying back to zero. To account for different plasma geometries and currents, the ohmic heating coil locations relative to the plasma centre scale with the TF coil radius and with the plasma major radius, and the current per turn scales linearly with the plasma current.

3.6.4 EF coils

The Equilibrium Field coils are based on the TITAN-I EF coils, which are two superconducting (NbTi) coils that provide the correct vertical field at the plasma centre. The coil locations scale with the plasma major radius and TF coil radius along with the ohmic heating coils.

3.6.5 Divertor

The TITAN divertor concept uses three poloidal divertors, which bear little resemblance to the typical tokamak toroidal divertor systems. The code uses the TITAN divertor lifetime of one year to enable the divertor costs to be reasonable, although the divertor surface area (and therefore the cost per divertor) is likely to be inaccurate.

3.6.6 Code modifications

As with the stellarator model, the RFP model has been incorporated in such a way as to allow its simple removal again if required in the future. All new routines are confined to the dedicated source file `rfp.f90`. The tokamak-relevant consistency equations in `PROCESS` (see Section 2.5) are used without modification, to ensure that the coil currents and the fields they produce are consistent with the plasma parameters.

3.7 Inertial Fusion Energy Model

As well as magnetic confinement devices, `PROCESS` has the ability to model inertial fusion plants, in which a laser or ion beam is used to ignite a target pellet containing the fusion fuel.

To activate the inertial fusion energy (IFE) coding, it is necessary to create a file `device.dat`, containing the single character `3` in the first row, in the working directory (see Section 4.4). This has the effect of setting the internally-used switch `ife = 1`. If the file is absent, or its first character is set to something other than `3`, the IFE model is not used, and `ife` is set to `0`.

The IFE model [54] is controlled using two additional switches.

`ifetyp = 0 :` Generic device build

`ifetyp = 1 :` OSIRIS-type device build [55, 56, 57]

`ifetyp = 2 :` SOMBRERO-type device build [58, 59]

`ifetyp = 3 :` HYLIFE-II-type device build [60, 61, 62]

Switch `ifetyp` defines the type of device that is assumed; this varies widely between different conceptual designs. The generic type assumes a cylindrically symmetric device, while the other types are approximations to the builds of the given conceptual machines [63]. In general, the build from the centre of the device (at the target ignition location) is in the order: chamber, first wall, gap, blanket, gap, shield, gap, building wall. The user specifies the thicknesses of these regions, and also the materials that are present and in what proportions.

`ifedrv = -1 :` Driver efficiency and target gain are input as functions of driver energy

`ifedrv = 0 :` Driver efficiency and target gain are input

`ifedrv = 1 :` SOMBRERO laser drive efficiency and target gain assumed

`ifedrv = 2 :` OSIRIS heavy ion beam driver efficiency and target gain are assumed [64]

Switch `ifedrv` defines how the code calculates the driver efficiency and target gain — these are the primary outputs required from the physics part of the model. For the SOMBRERO and OSIRIS cases (`ifedrv = 1` and `ifedrv = 2`, respectively) the driver efficiency and gain are calculated from curves of these parameters as functions of the driver energy. For the `ifedrv = -1` case, the user provides the driver efficiency and target gain versus driver energy, via the two arrays `etave(1:10)` and `gainve(1:10)` respectively; the element number corresponds to the driver energy in MJ, and outside the range 1–10 MJ the curves are extrapolated linearly. Finally, for the `ifedrv = 0` case, the user inputs single values for the driver efficiency (`drveff`) and target gain (`tgain`).

Constraint equation no. 50 can be turned on to enable the ignition repetition rate to remain below a user-specified upper limit (`rrmax`); iteration variable no. 86 (`frrmax`) is the associated f-value (see Section 2.5). The other iteration variables relevant for the IFE model are nos. 81–85 (`edrive`, `drveff`, `tgain`, `chrad` and `pdrive` — see Table 2.2).

3.8 Safety and Environment Models

At present, the neutronics, activation and inventory calculations comprise the safety and environment models in the code.

The models comprising the safety and environmental calculations [65] within the code are all called from routine `FISPAC`. They are only performed once, at the end of each run, as they take a relatively long time to evaluate, and the results are only used for diagnostic purposes — no constraints are imposed at present to minimise doses, for instance.

N.B. These models are currently not available in the present version of the code.

3.8.1 Neutronics

The neutronics module predicts the neutron flux spectra in the inboard and outboard first wall and blanket components. The spectra are based on a simplified tokamak device that has a fixed ratio (= 1.5825) between the outboard blanket thickness and the inboard blanket thickness, and are scaled according to the actual thickness of the outboard blanket. This relatively limited, single-parameter approach is expected to be replaced by a more general method, which should allow a more accurate portrayal of the device being modelled by `PROCESS`.

3.8.2 Activation and inventory information

The code evaluates the consequences of exposing the power plant's materials to the calculated neutron fluxes, subject to the limitations imposed by the neutronics module. A library of neutron cross-sections and decay data is used to calculate the total activity, gamma-ray dose rate and decay heat output due to the materials' exposure to neutrons, both at the end of the plant's life and at a time 100 years later. These values are relevant to decommissioning and disposal studies, and additional parameters that can be obtained from the nuclide inventory will also be included as the need arises.

3.9 Cost Models

Two cost models are available, determined by the switch `cost_model`.

3.9.1 1990 cost model (`cost_model = 0`)

This combines methods [66] used in the TETRA code [1] and the Generomak [67] scheme. The costs are split into accounting categories [68]. The best references for the algorithms used are [2], and source file `costs.f90` in the code itself. The majority of the costed items have a unit cost associated with them. These values scale with (for example) power output, volume, component mass etc., and many are available to be changed via the input file. All costs and their algorithms correspond to 1990 dollars.

The unit costs of the components of the fusion power core are relevant to "first-of-a-kind" items. That is to say, the items are assumed to be relatively expensive to build as they are effectively prototypes and specialised tools and machines have perhaps been made specially to create them. However, if a "production line" has been set up, and R & D progress has allowed more experience to be gained in constructing the power core components, the costs will be reduced as a result. Variable `fkind` may be used to multiply the raw unit costs of the fusion power core items (by a factor less than one) to simulate this cost reduction for an Nth-of-a-kind device. In other systems studies of fusion power plants [69], values for this multiplier have ranged from 0.5 to 0.8.

Many of the unit costs have four possible choices, relating to the level of safety assurance [70] flag `lsa`. A value `lsa = 1` corresponds to a plant with a full safety credit (i.e. is truly passively safe). Levels `2` and `3` lie between the two extremes, and level `4` corresponds to a present day fission reactor, with no safety credit.

The first wall, blanket, divertor, centrepost (if present) and current drive system have relatively short lifetimes because of their hostile environment, after which they must be replaced. Because of this frequent renewal they can be regarded as though they are "fuel" items, and can be costed accordingly. Switch `ifueltyp` is used to control whether this option is used in the code. If `ifueltyp = 1`, the costs of the first wall, blanket, divertor and a fraction `fcdfuel` of the cost of the current drive system are treated as fuel costs. If `ifueltyp = 0`, these are treated as capital costs.

If the switch `ireactor = 0`, no cost of electricity calculation is performed. If `ireactor = 1`, then the cost of electricity is evaluated, with the value quoted in units of $/MWh.

The net electric power is calculated in routine `POWER`. It is possible that the net electric power can become negative due to a high recirculating power. Switch `ipnet` determines whether the net electric power is scaled to always remain positive (`ipnet = 0`), or whether it is allowed to become negative (`ipnet = 1`), in which case no cost of electricity calculation is performed.

3.9.2 2015 Kovari model (`cost_model = 1`)

This model [21] provides only capital cost, and is not currently suitable for estimating the cost of electricity. N^{th}-of-a-kind factors, level of safety assurance factors, and blanket replacement costs are not included. The mean electric output is calculated using the capacity factor, which takes accountof the availability and the dwell time for a pulsed reactor. The capital cost divided by the mean electric output is a useful comparison parameter.

3.10 Plant availability

Switch `iavail` is used to control how the overall plant availability factor `cfactr` is calculated, as follows

If `iavail = 0`, the input value of cfactr is used.

If `iavail = 1`, a model by N. Taylor and D. Ward [71] is used instead, in which `cfactr` is calculated taking into account the time taken to replace certain components of the fusion power core, and various unplanned unavailability fractions which may be set by the user, as summarised in Table 3.5.

input parameter	description
`tbktrepl`	time needed to replace blanket (years)
`tdivrepl`	time needed to replace divertor (years)
`tcomrepl`	time needed to replace both blanket and divertor (years)
`uubop`	unplanned unavailability of balance of plant
`uucd`	unplanned unavailability of current drive system
`uudiv`	unplanned unavailability of divertor
`uufuel`	unplanned unavailability of fuelling system
`uufw`	unplanned unavailability of first wall
`uumag`	unplanned unavailability of magnets
`uuves`	unplanned unavailability of vessel

Table 3.5: *Summary of the variables in PROCESS that relate to the Taylor-Ward availability model (`iavail=1`).*

If `iavail = 2`, the new Morris model is implemented [20]. It estimates both planned and unplanned unavailability, and the time during which no power is being generated if the reactor is pulsed.

The planned unavailability is linked to the lifetimes of the blanket and divertor and the time taken to replace them. The lifetime of the blanket is based on the allowable fast neutron fluence. In contrast, the lifetime of the divertor is estimated using the particle and photon load. The time to replace the blanket and divertor have been estimated by Crofts et al, who studied the influence of the number of remote handling systems working in parallel. `PROCESS` uses a simple fit to their results, and adds a month to allow the dose rate to reduce to an acceptable level before remote handling operations start, and a month to allow for pump-down and preparation for operation at the end of the shutdown.

To estimate the unplanned downtime, each susbsystem is represented by a simple model that tries to capture the degradation of reliability when approaching operational and technological limits. This increases the risk of unplanned downtime as design margins are reduced.

For the toroidal field coils, the chance of a quench is likely to be the largest driver of the risk of unplanned unavailability, and this may depend on the temperature margin - the difference between the

actual temperature and the critical temperature of the superconductor. The user inputs a minimum temperature margin, below which quench is immediate, and a second, higher value, above which quenches never occur. In between, there is a finite quench rate.

The unplanned downtime for the blanket is based on the number of cycles it experiences before planned replacment. (This model is restricted to pulsed reactors.) The cycle life of the blanket is expressed using a reference lifetime. Before this liefetime, there is a constant but small probability of failure in ecah pulse. After the reference lifetime the reliability of the blanket starts to decline, reaching zero at the upper lifetime limit.

It is assumed that the vacuum system can be maintained in parallel with blanket replacement, so it does not contribute to the planned downtime. The unplanned downtime is based on an assumed failure rate for a cryopump, and a specified total number of pumps, with some of them being redundant. The resulting downtime can be reduced to a negligible level if there are several redundant pumps, but in addition, there is a fixed unavailability to allow for common mode failures affecting several pumps.

Chapter 4

Running PROCESS

The intention of this chapter is to provide a comprehensive prescription for setting up and performing runs with the code. Firstly, the input file's structure and format is described. The user is then taken through the procedure for setting up the code to model a new machine, and finally an attempt is made to indicate and solve the problems that the user will face whilst trying to achieve a feasible solution.

4.1 Environment set-up

PROCESS is available for execution from the CCFE Fusion Unix Network, on which you must have an account.

To set up your environment to be able to run the code, the user interface and the associated utilities (see Chapter 6), add the following lines to your .bashrc file. This is a file in the user's home directory, assuming the bash Unix shell is being used. Although hidden, it can be opened by issuing the relevant command, for example gedit .bashrc.

```
module use /home/PROCESS/modules
module swap python
module load process/master
```

(If you want to use the latest draft version of the code instead of the latest verified release version, replace module load process/master with module load process/develop above.)

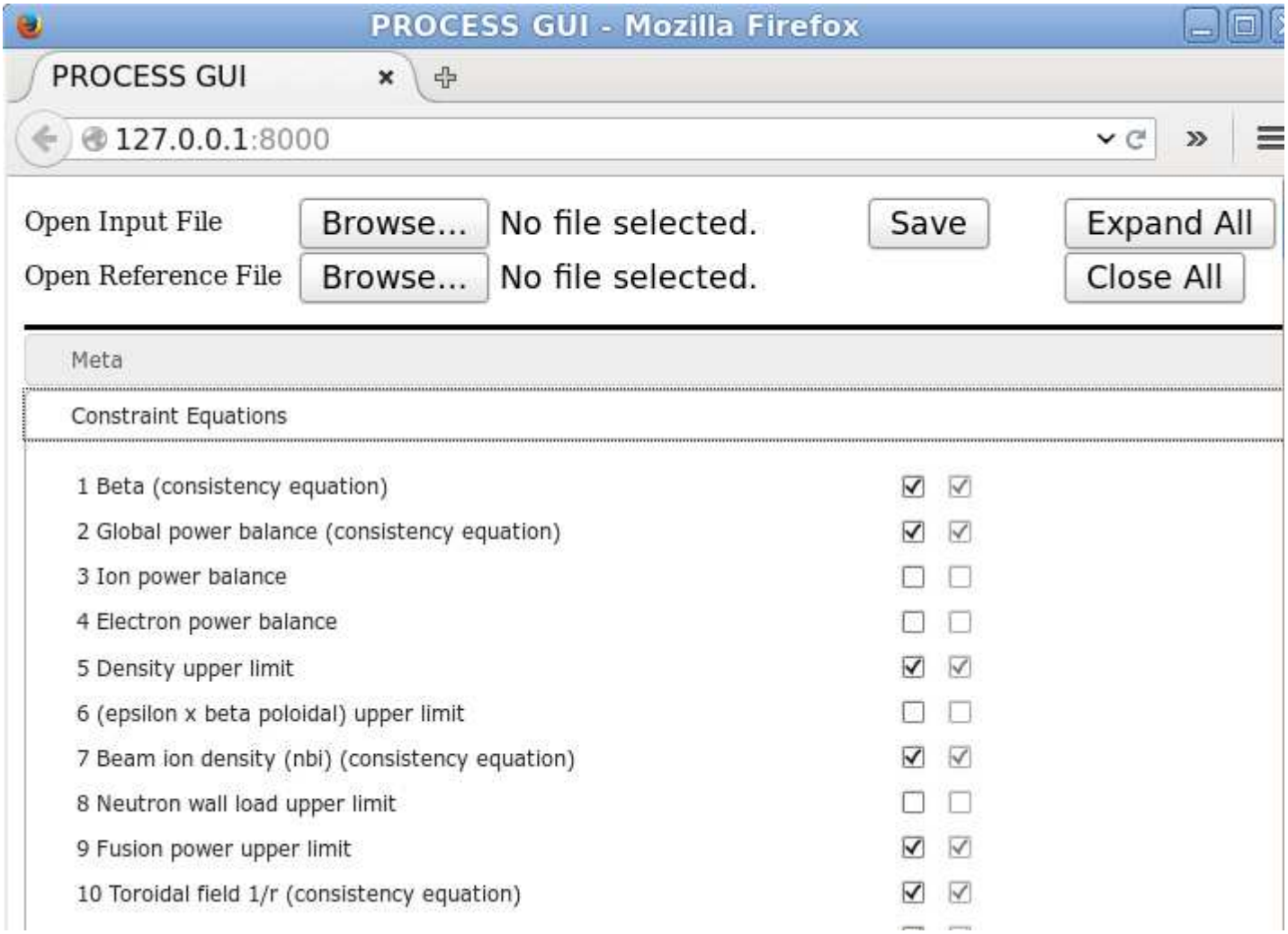
4.2 User Interface

The user interface allows for viewing and editing of IN.DAT files in a web browser. Launch the interface (GUI) by typing start_gui from the Unix command line.

(The interface uses Django for its web framework. Currently it can only be launched by running the Django development server locally. This is performed automatically if you launch the GUI as above. For instructions on starting the server manually, see the README file in the utilities/processgui directory.)

Please note: If you are working on a Linux desktop machine and already have Firefox open, typing start_gui *on a Fusion Unix Network machine will try to open a PROCESS GUI session on the already-open Firefox running locally. This will fail! You need to either close the local Firefox session completely*

before typing `start_gui` *or open a different browser manually (e.g. konqueror) after typing* `start_gui` *and navigate to 127.0.0.1:8000 in the address bar.*



Every variable is listed along with its current value, a 'reference' value and a short description. Hovering over the short description will provide a longer description. Until an input file is opened, all values are given their default values assigned by `PROCESS`.

The reference values are used to compare differences between two files. Differences between the reference value and the current input value will be highlighted in red.

The 'Meta' section allows editing of the run description, which will be placed at the top of the created `IN.DAT`. Iteration variables and constraint equations can be enabled using the checkboxes in the relevant sections.

An input file and a reference file can be opened using the buttons at the top of the window. The files opened must be compatible with the `PROCESS` version number shown in the top right of the window.

The 'Save' button creates an `IN.DAT` file with a similar layout to the GUI. Variables whose values are set different from the `PROCESS` default are listed under module headings, along with a comment describing the variable. For integer variables, a description of the value selected may also be included. The variables `neqns` (number of constraints) and `nvar` (number of iteration variables) are automatically calculated.

When using the Firefox web browser it can save time to select

`Preferences > General > Downloads > Always ask me where to save files.`

You can searching for a particular variable can be done using the browser's in-built search. Use the "Expand" button in the top-right of the window to expand every module heading and use Ctrl-f to search.

4.3 Executing the Code

Execute PROCESS by simply typing `process` on the Unix command line.

By default, the input and output file names are as described in the following sections. If, however, PROCESS is executed with an argument, this is used as a prefix to the file names:

```
process myrun
```

will assume that the input file is called *myrun*IN.DAT, etc.

The input file must be in the current directory. The output files *myrun*OUT.DAT and *myrun*MFILE.DAT will be created in the current directory.

4.4 The Input File

The input file IN.DAT is used to change the values of the physics, engineering and other code parameters from their default values, and to set up the numerics (constraint equations, iteration variables etc.) required to define the problem to be solved. The user interface writes the input file, so it is not necessary to edit it directly. Details of layout and format are in Appendix B.

If the code encounters a problem reading the input file, it will stop immediately with an error message. The last line of the output file OUT.DAT may give an indication of where in the input file the problem lies.

4.5 The Output Files

The main output from the code is sent to file OUT.DAT in the working directory. It is essential to check that the code reports that it has found a *feasible solution*.

A second file, MFILE.DAT, is also produced in the working directory. This file contains most of the same data as OUT.DAT but in a different format, and has been designed to be "machine-readable" by some of the utility programs described in Chapter 6, to allow simple post-processing and graphical output to be produced easily.

4.6 Optimisation mode

Switch `ioptimz` should be set to `1` for optimisation mode.

If `ioptimz = 0`, a non-optimisation pass is performed first. Occasionally this provides a feasible set of initial conditions that aids convergence of the optimiser, but it is recommended to use `ioptimz = 1`.

Enable all the relevant consistency equations, and it is advisable to enable the corresponding iteration variables shown in bold in Table 2.3. A number of limit equations (inequality constraints) can also be activated. For limit equations, the corresponding f-value must be selected as an iteration variable. In optimisation mode, the number of iteration variables is unlimited.

It may still be difficult, if not impossible, to reconcile the fusion power and the net electric power with the required values. This may well be due to the power conversion efficiency values being used — refer to Figure 3.9.

With luck, a few iterations of this process will produce an adequate benchmark case. A typical input file for use with PROCESS in non-optimisation mode is contained in Appendix D.

If scans of a given variable are to be made over a large range of values, it is often a good idea to start the scan in the middle of the desired range, and to split the scan in two — one going downwards from the initial value, and the other upwards. This ensures that the whole range of the scan produces well-converged machines (assuming a "good" initial point), without sharp changes in gradient in the parameter values.

It should be remembered that the value of the scan variable is set in the array `sweep`, and this overrules any value set for the variable elsewhere in the input file.

The output from an optimisation run contains an indication as to which iteration variables lie at their limiting values. A typical input file for use with PROCESS in optimisation mode is contained in Appendix C.

4.7 Non-optimisation mode

Non-optimisation mode is sometimes used to perform benchmark comparisons, whereby the machine size, output power etc. are known and one only wishes to find the calculated stresses, beta values and fusion powers, for example.

Running PROCESS in non-optimisation mode requires few changes to be made to the input file from the non-optimisation case. The main differences between optimisation mode and non-optimisation mode are:

1. Non-optimisation mode does NOT apply lower or upper bounds to the iteration variables. It follows that limit equations are not enforced.
2. In non-optimisation mode the number of active iteration variables must be equal to the number of constraints.
3. A figure of merit is not available in non-optimisation mode.
4. Scans cannot be performed in non-optimisation mode.

As before, the user must decide which constraint equations and iteration variables to activate.

4.8 Troubleshooting

Experience has shown that the first few attempts at running PROCESS with a new input file tends to produce unfeasible results — that is, the code will not find a consistent set of machine parameters. The highly non-linear nature of the numerics of PROCESS is the reason for this difficulty, and it often

requires a great deal of painstaking adjustment of the input file to overcome. The utility a_to_b (subsection 6.1.12) is useful in this situation.

4.8.1 Error handling

In general, errors detected during a run are handled in a consistent manner, with the code producing (hopefully) useful diagnostic messages to help the user understand what has happened.

There are three levels of errors and warning that may occur:

Level 1: An *informational* message is produced under certain conditions, for example if the code has modified the user's input choice for some reason.

Level 2: A *warning* message is produced if a non-fatal situation has occurred that may result in an output case that is inaccurate or unreliable in some way.

Level 3: An *error* message will occur if a severe or fatal error has occurred and the program cannot continue.

These messages are printed on the screen during the course of a run, and those still active at the final (feasible or unfeasible) solution point are also written to the end of the output file (messages encountered during the iteration process are not copied to the output file, as the convergence to a valid solution might resolve some of the warnings produced earlier in the solution process).

The error_status variable returns the highest severity level that has been encountered (or zero if no abnormal conditions have been found); if a severe error (level 3) is flagged at any point the program is terminated immediately. The final message number encountered during a run is returned via output variable error_id. In addition, with certain messages, a number of diagnostic values may also be given; these can be used to provide extra diagnostic information if the source code is available.

4.8.2 General problems

A code of the size and complexity of PROCESS contains myriads of equations and variables. Virtually everything depends indirectly on everything else because of the nature of the code structure, so perhaps it is not surprising that it is often difficult to achieve a successful outcome.

Naturally, problems will occur if some of the parameters become unphysical. For example, if the aspect ratio becomes less than or equal to one, then we must expect problems to appear. For this reason, the bounds on the iteration variables should be selected with care.

Occasionally arithmetic ("NaN") errors are reported. They usually occur when the code is exploring unphysical values of the parameters, and often suggest that no feasible solution exists for the input file used.

The error messages produced by the code attempt to provide diagnostic information, telling the user where the problem occurs, and also suggest a possible solution. These messages are out of necessity brief, and so cannot promise to lead to a more successful outcome.

There is the option to turn on extra debugging output; to do this, set verbose = 1 in the input file.

4.8.3 Optimisation problems

On reflection it is perhaps surprising that PROCESS ever does manage to find the global minimum figure of merit value, since if there are nvar iteration variables active the search is over nvar-

dimensional parameter space, in which there may be many shallow minima of approximately equal depth. Remember that `nvar` is usually of the order of twenty.

The machine found by `PROCESS` may not, therefore, be the absolutely optimal device. It is quite easy to have two or more solutions, with results only a few per cent different, but a long way apart in parameter space. The technique of "stationary" scans is sometimes used in this situation: a scan is requested, but the same value of the scan variable is listed repeatedly.

Scans should be started in the middle of a range of values, to try to keep the scan within the same family of machines. The optimum machine found may otherwise suddenly jump to a new region of parameter space, causing the output variables to seem to vary unpredictably with the scanning variable.

It should be noted that in general the machine produced by `PROCESS` will always sit against one or more operation limits. If, during a scan, the limit being leant upon changes (i.e. if the machine jumps from leaning on the beta limit to leaning on the density limit) the output parameters may well become discontinuous in gradient, and trends may suddenly change direction.

4.8.4 Unfeasible results

In the numerics section of the output file, the code indicates whether the run produced a feasible or unfeasible result.

The former implies a successful outcome, although it is always worth checking that the sum of the squares of the constraint residuals (`sqsumsq`) is small ($\sim 10^{-3}$ or less); the code will issue a warning if the solver reports convergence but the value of `sqsumsq` exceeds 10^{-2}. If this occurs, reducing the value of the HYBRD tolerance `ftol` or `VMCON` tolerance `epsvmc` as appropriate should indicate whether the result is valid or not; the output can usually be trusted if (1) the constraint residues[1] fall as the tolerance is reduced to about 10^{-8}, and (2) the code indicates that a feasible solution is still found.

An unfeasible result occurs if `PROCESS` cannot find a set of values for the iteration variables which satisfies all the given constraints. In this case, the values of the constraint residues shown in the output give some indication of which constraint equations are not being satisfied — those with the highest residues should be examined further. In optimisation mode, the code also indicates which iteration variables lie at the edge of their allowed range.

Unfeasible runs can be caused by specifying physically incompatible input parameters, using insufficient iteration variables, or by starting the problem with unsuitable values of the iteration variables.

The utility `run_process` (Section 6.1.2) carries out many runs, changing the starting values of the iteration variables randomly. It stops once a feasible solution is found.

Another approach is to start with an input file that gives a feasible solution, and modify it step by step towards the parameters desired. This process is automated by the utility `a_to_b` ((Section 6.1.12).

It is important to choose the right number of *useful* iteration variables for the problem to be solved — it is possible to activate too many iteration variables as well as too few, some of which may be redundant.

Both optimisation and non-optimisation runs can fail with an error message suggesting that the iteration process is not making good progress. This is likely to be due to the code finding itself unable to escape a region of the parameter space where the minimum in the residuals is significantly above

[1] The constraint residues are the final values of c_i in the constraint equations — see Section 2.5. The value `sqsumsq` is the square root of the sum of the squares of these residuals.

zero. In this situation, there is either no solution possible (the residuals can therefore never approach zero), or the topology of the local minimum makes it difficult for the code to escape to the global minimum. Again, a helpful technique is to either change the list of iteration variables in use, or to simply modify their initial values to try to help the code avoid such regions.

A technique that occasionally removes problems due to unfeasible results, particularly if an error code `ifail = 3` is encountered during an optimisation run, is to adjust slightly one of the limits imposed on the iteration variables, even if the limit in question has not been reached. This subtly alters the gradients computed by the code during the iteration process, and may tip the balance so that the code decides that the device produced is feasible after all. For instance, a certain component's temperature might be 400 K, and its maximum allowable temperature is 1000 K. Adjusting this limit to 900 K (which will make no difference to the *actual* temperature) may be enough to persuade the code that it has found a feasible solution.

Similarly, the order in which the constraint equations and iteration variables are stored in the `icc` and `ixc` arrays can make the difference between a feasible and unfeasible result. This seemingly illogical behaviour is, sadly, typical of the way in which the code works.

Another technique in such situations may be to change the finite difference step length `epsfcn`, as this might subtly change the path taken in the approach towards a solution.

It may be the case that the act of satisfying all the required constraints is impossible. No machine can exist if the allowed operating regime is too restrictive, or if two constraint equations require conflicting (non-overlapping) parameter spaces. In this case some relaxation of the requirements is needed for the code to produce a successful machine design.

4.8.5 Hints

The above sections should indicate that it is the complex interplay between the constraint equations and the iteration variables that determines whether the code will be successful at producing a useful result. It can be a somewhat laborious process to arrive at a working case, and (unfortunately, perhaps) experience is often of great value in this situation.

It should be remembered that sufficient iteration variables should be used to solve each constraint equation. For instance, a particular limit equation may be $A \leq B$, i.e. $A = fB$, where the f-value f must lie between zero and one for the relation to be satisfied. However, if none of the iteration variables have any effect on the values of A and B, and A happens to be *greater* than B, then `PROCESS` will clearly not be able to solve the constraint.

The lower and upper bounds of the iteration variables are all available to be changed in the input file. Constraints can be relaxed in a controlled manner by moving these bounds, although in some cases care should be taken to ensure that unphysical values cannot occur. The code indicates which iteration variables lie at the edge of their range.

It is suggested that constraint equations should be added one at a time, with sufficient new iteration variables activated at each step. If the situation becomes unfeasible it can be helpful to reset the initial iteration variable values to those shown in the output from a previous feasible case, and rerun the code.

Chapter 5

Changing the Source Code: New Models, Variables and Constraints

It is often useful to add extra features to the code in order to model new situations. This chapter provides instructions on how to do this, with specific details on how to add various numerics related items to `PROCESS`.

Please remember to modify the relevant sections and table(s) in this User Guide if changes are made to the source code!

5.1 Source Code Modification

Described here are the general rules that apply when the Fortran source code is modified. See Section 7.3 for instructions on how to commit changes to the `PROCESS` Git repository and produce new releases. The variable descriptor file is generated from specially-formatted comment lines within the source code (see Section 7.2 for more details). Therefore, it is exceedingly important to keep these lines relevant and in sync with the variables they describe.

5.1.1 Changing the Fortran code

Please ensure that the following rules are adhered to when modifying the `PROCESS` source code:

1. Keep the layout consistent in with the existing code, including indentation of clauses (`if`-statements, `do`-loops, etc.).
2. Use the standard routine header (see below).
3. Always use `implicit none` and declare all local variables explicitly.
4. Declare all 'real' (i.e. floating-point) variables as `real(kind(1.0D0))`.
5. Ensure all routine arguments have the appropriate attribute `intent(in)`, `intent(out)` or `intent(inout)`, as necessary.
6. Always write explicit real constants using the scientific `D` notation, e.g. `1.0D0`, `2.3D0`, `-1.23D6`. That is to say, use `1.0D0` and not `1.0` or `1.` or `1` when the expression should be using floating-point arithmetic.

A Fortran 90/95 manual, complete with guidelines for good Fortran 90/95 practice, may be found at the following webpage:

`http://fusweb1.fusion.ccfe.ac.uk/~pknight/f95notebook.html`

5.1.2 Source code documentation

It is critically important to keep the documentation in the source code itself up-to-date, relevant and tidy. Please keep to the following guidelines whenever the source code is modified.

1. Use comments copiously in the code.
2. Use the standard header layout, and do not omit any of the sections. Here is an example subprogram header:

```
! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

subroutine culblm(bt,dnbeta,plascur,rminor,betalim)

  !+ad_name  culblm
  !+ad_summ  Beta scaling limit
  !+ad_type  Subroutine
  !+ad_auth  P J Knight, CCFE, Culham Science Centre
  !+ad_cont  N/A
  !+ad_args  bt      : input real :  toroidal B-field on plasma axis (T)
  !+ad_args  dnbeta  : input real :  Troyon-like g coefficient
  !+ad_args  plascur : input real :  plasma current (A)
  !+ad_args  rminor  : input real :  plasma minor axis (m)
  !+ad_args  betalim : output real : beta limit as defined below
  !+ad_desc  This subroutine calculates the beta limit, using
  !+ad_desc  the algorithm documented in AEA FUS 172.
  !+ad_desc  <P>The limit applies to beta defined with respect to the total B-field.
  !+ad_desc  Switch ICULBL determines which components of beta to include (see
  !+ad_desc  routine <A HREF="constraints.html">constraints</A> for coding):
  !+ad_desc  <UL>
  !+ad_desc  <P><LI>If ICULBL = 0, then the limit is applied to the total beta
  !+ad_desc  <P><LI>If ICULBL = 1, then the limit is applied to the thermal beta only
  !+ad_desc  <P><LI>If ICULBL = 2, then the limit is applied to the thermal +
  !+ad_desc                        neutral beam beta components
  !+ad_desc  </UL>
  !+ad_desc  The default value for the g coefficient is DNBETA = 3.5
  !+ad_prob  None
  !+ad_call  None
  !+ad_hist  21/06/94 PJK Upgrade to higher standard of coding
  !+ad_hist  09/11/11 PJK Initial F90 version
  !+ad_hist  27/06/13 PJK Modified header comments
  !+ad_stat  Okay
  !+ad_docs  AEA FUS 172: Physics Assessment for the European Reactor Study
  !+ad_docs  AEA FUS 251: A User's Guide to the PROCESS Systems Code
  !
  ! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

   A description of all the available automatic documentation marker tags (these all start with `!+ad_`) may be found by examining the main program header of the (self-documenting!) automatic documentation program itself (in file `autodoc.f90`).

3. After **every** change within a routine, add a new history line (using `!+ad_hist`, and `!+ad_hisc` for continuation lines) to its header. Ensure that all routines called are listed via `!+ad_call`

lines. Update the description lines as necessary. You may use html tags and hyperlinks (some are shown in the example above) as required; to be sure that they have been added correctly, type `make html` to create the web documentation and examine the relevant html file (i.e. `culblm.html` for the example above) using your favourite web browser.

4. If you add a new routine to a module, remember to modify the header of the module as well as that of the new routine (add a `!+ad_cont` line to it).

5. Add suitable documentation to this User Guide whenever a model is added or modified. This should be done immediately to ensure that the Guide remains consistent with the source code. Change the code's revision number and the date in `process.tex`.

6. Add a new file to the folder `release_notes`. It is particularly important to describe here any changes to the required IN.DAT - especially any change that makes previous IN.DAT files unusable.

5.2 Input Parameters

Input parameters (see Section 2.3) are added to the code in the following way:

1. Choose the most relevant module (usually one of those in source file `global_variables.f90`). Keeping everything in alphabetical order (or possibly within a group of variables closely-related to a particular switch), add a declaration statement for the new variable, specifying a "sensible" default value, and a correctly formatted comment line to describe the variable. Copy the examples already present, such as

```
!+ad_vars  abktflnc /5.0/ : allowable first wall/blanket neutron
!+ad_varc                   fluence (MW-yr/m2) (blktmodel=0)
real(kind(1.0D0)) :: abktflnc = 5.0D0
```

   Note that the automatic documentation marker tag `!+ad_vars` tells the `autodoc` utility (Section 7.2) that the line is (the first line of) a variable description, while `!+ad_varc` specifies any continuation lines. Also note that the colon (:) on the first line is necessary, as it is assumed to exist by the dictionary-building Python utility for the GUI.

2. Add a dated comment (using `!+ad_hist`) to the header of the relevant module.

3. Ensure that all the modules that use the new variable reference the relevant module via the Fortran `use` statement.

4. Add the parameter to routine `PARSE_INPUT_FILE` in source file `input.f90` in a suitable place — keep to alphabetical order. The existing examples provide guidance on how to do this. Note that real (i.e. double precision) and integer variables are treated differently, as are scalar quantities and arrays.

5.3 Iteration Variables

New iteration variables (see Section 2.4) are added in the same way as input parameters, with the following additions:

1. Increment the parameter `ipnvars` in module `numerics` in source file `numerics.f90` in order to accommodate the new iteration variable.
2. Add an additional line to the initialisation of the array `ixc` in module `numerics` in source file `numerics.f90`.
3. Assign sensible values for the variable's bounds to the relevant elements in arrays `boundl` and `boundu` in module `numerics` in source file `numerics.f90`.
4. Assign the relevant element of character array `lablxc` to the name of the variable, in module `numerics` in source file `numerics.f90`.
5. Add the variable to routines `LOADXC` and `CONVXC` in source file `iteration_variables.f90`, mimicking the way that the existing iteration variables are coded.
6. Modify the variable's description in its declaring module (which is likely to be in source file `global_variables.f90`), to say that it is "(iteration variable XXX)"
7. Add dated comments (using `!+ad_hist`) to the headers of all affected routines and modules.
8. Modify Table 2.2 of this User Guide (`UserGuide_Chapter2.tex`).

If an existing input parameter is now required to be an iteration variable, then simply carry out the tasks mentioned here.

It should be noted that iteration variables must not be reset elsewhere in the code. That is, they may only be assigned new values when originally initialised (in the relevant module, or in the input file if required), and in routine `CONVXC` where the iteration process itself is performed. Otherwise, the numerical procedure cannot adjust the value as it requires, and the program will fail.

5.4 Other Global Variables

This type of variable embraces all those present in the modules in `global_variables.f90` (and some others elsewhere) which do not need to be given initial values or to be input, as they are calculated within the code. These should be added to the code in the following way:

1. Choose the most relevant module (usually one of those in source file `global_variables.f90`). Keeping everything in alphabetical order (or possibly within a group of variables closely-related to a particular switch), add a declaration statement for the new variable, specifying the initial value `0.0D0`, and a correctly formatted comment line to describe the variable (copying the examples already present — see also "Input Parameters" above).
2. Ensure that all the modules that use the new variable reference the relevant module via the Fortran `use` statement.

5.5 Constraint Equations

Constraint equations (see Section 2.5) are added to `PROCESS` in the following way:

1. Increment the parameter `ipeqns` in module `numerics` in source file `numerics.f90` in order to accommodate the new constraint.

2. Add an additional line to the initialisation of the array `icc` in module `numerics` in source file `numerics.f90`.

3. Assign a description of the new constraint to the relevant element of array `lablcc`, in module `numerics` in source file `numerics.f90`.

4. Add a new Fortran `case` statement containing the new constraint equation to routine `CONSTRAINT_EQNS` in source file `constraint_equations.f90`, ensuring that all the variables used in the formula are contained in the modules specified via `use` statements present at the start of this file. Use a similar formulation to that used for the existing constraint equations, remembering that the code will try to force `cc(i)` to be zero.

5. Add dated comments (using `!+ad_hist`) to the headers of all affected routines and modules.

6. Modify Table 2.4 of this User Guide (`UserGuide_Chapter2.tex`).

Remember that if a limit equation is being added, a new f-value iteration variable may also need to be added to the code.

5.6 Figures of Merit

New figures of merit (see Section 2.6) are added to `PROCESS` in the following way:

1. Increment the parameter `ipnfoms` in module `numerics` in source file `numerics.f90` to accommodate the new figure of merit.

2. Assign a description of the new figure of merit to the relevant element of array `lablmm` in module `numerics` in source file `numerics.f90`.

3. Add the new figure of merit equation to routine `FUNFOM` in source file `evaluators.f90`, following the method used in the existing examples. The value of `fc` should be of order unity, so select a reasonable scaling factor if necessary. Ensure that all the variables used in the new equation are contained in the modules specified via `use` statements present at the start of this file.

4. Add dated comments (using `!+ad_hist`) to the headers of all affected routines and modules.

5. Modify Table 2.5 of this User Guide (`UserGuide_Chapter2.tex`).

5.7 Scanning Variables

Scanning variables (see Section 2.7) are added to `PROCESS` in the following way:

1. Increment the parameter `ipnscnv` in module `scan_module` in source file `scan.f90` to accommodate the new scanning variable.

2. Add a short description of the new scanning variable to the `nsweep` entry in source file `scan.f90`.

3. Add a new assignment to the relevant part of routine `SCAN` in source file `scan.f90`, following the examples already present, including the inclusion of a short description of the new scanning variable in variable `xlabel`.

4. Ensure that the scanning variable used in the assignment is contained in one of the modules specified via `use` statements present at the start of this routine.
5. Add dated comments (using `!+ad_hist`) to the headers of all affected routines and modules.
6. Modify Table 2.6 of this User Guide (`UserGuide_Chapter2.tex`).

5.8 Submission of New Models

The `PROCESS` source code is maintained by CCFE, and resides in a *Git* [72] repository on the CCFE servers. We welcome contributions of alternative or improved models and algorithms.

We request that contributors provide the following information for any new models that they provide:

- A comprehensive description of the model; please provide a full list of references.
- A list of all inputs and outputs: descriptions, default (input) values, allowed ranges, units.
- If possible, please cross-reference any input/output variables to existing global variables listed in the variable descriptor file (see Section 2.2).
- Any new input parameters, iteration variables, constraint equations, figures of merit etc.
- A definition of any pre-requisites.
- Any available test data, code examples or test programs in any language.

5.9 Code Structure

5.9.1 Numerics modules

These modules contain the equation solvers, their calling routines and other relevant procedures. Various mathematical routines from a number of standard libraries are also incorporated into these files. Table 5.1 summarises the numerics source files.

source file	description
`caller.f90`	calls physics, engineering, building and cost routines
`constraint_equations.f90`	defines the constraint equations
`evaluators.f90`	function evaluators for HYBRD and `VMCON` packages
`iteration_variables.f90`	adjusts values of iteration variables
`maths_library.f90`	miscellaneous 'black-box' maths routines, including HYBRD and `VMCON`
`numerics.f90`	numerics array definitions, and calling routines for HYBRD and `VMCON` packages
`scan.f90`	performs a parameter scan

Table 5.1: *Summary of the numerics modules in `PROCESS`.*

5.9.2 Physics modules

These modules contain the main physics routines that evaluate the plasma and fusion parameters. Also included here are the routines describing the current drive and divertor systems. Table 5.2 summarises the main physics source files.

source file	description
`current_drive.f90`	current drive efficiency calculations
`divertor.f90`	divertor model calculations
`fispact.f90`	nuclide inventory/activation calculations
`ife.f90`	inertial fusion energy physics/engineering
`impurity_radiation.f90`	radiation power calculations
`physics.f90`	tokamak plasma and fusion calculations
`plasma_geometry.f90`	plasma geometry algorithms
`plasma_profiles.f90`	plasma density and temperature profile calculations
`rfp.f90`	reversed field pinch physics/engineering
`startup.f90`	plasma start-up auxiliary power requirements
`stellarator.f90`	stellarator-relevant physics/engineering

Table 5.2: *Summary of the physics modules in* `PROCESS`.

5.9.3 Engineering modules

These modules contain the description of the machine geometry and its major systems, including the PF and TF coil sets, the first wall, blanket and shield, and other items such as the buildings, vacuum system, power conversion and the structural components. Table 5.3 summarises the main engineering source files.

source file	description
`availability.f90`	plant component lifetimes and overall availability
`buildings.f90`	buildings calculations
`fwbs.f90`	first wall, blanket and shield calculations
`machine_build.f90`	machine build calculations
`pfcoil.f90`	PF coil calculations
`plant_power.f90`	heat transport and power balance calculations
`pulse.f90`	pulsed power plant calculations
`safety.f90`	steady-state temperatures after a LOCA event
`sctfcoil.f90`	superconducting TF coil calculations
`structure.f90`	support structure calculations
`tfcoil.f90`	resistive TF coil calculations
`vacuum.f90`	vacuum system calculations

Table 5.3: *Summary of the engineering modules in* `PROCESS`.

5.9.4 Costing module

The costing module, `costs.f90`, performs all the cost calculations, including values in M$ for each machine system, and the cost of electricity in m$/kWh. Normally, the machine costs are written to the output file; if this is not required set switch `output_costs = 0`.

5.9.5 Other modules

These modules perform miscellaneous tasks, such as initialisation of variables and file input / output. File `process.f90` contains the main program, and includes the overall controlling loop.

Table 5.4 summarises these modules.

source file	description
`error_handling.f90`	centralised error handling module
`fson_library.f90`	library used to read in data from JSON-format files
`global_variables.f90`	defines and initialises most shared variables
`initial.f90`	checks self-consistency of input variables and switches
`input.f90`	reads in user-defined settings from input file
`output.f90`	utility routines to format output to file
`process.f90`	main program and top-level calling routines

Table 5.4: *Summary of the remaining modules in* `PROCESS`.

Chapter 6

Utility Programs

A number of utilities for PROCESS are available, for instance to modify the input file IN.DAT, run PROCESS until a feasible solution is found, or to extract and plot data from the PROCESS output. All utilities are available from PROCESS/master/utilities.

For PROCESS *users*, only the executables described in Section 6.1 are relevant. For anyone interested in modifying the existing code or developing new utilities the PROCESS Python libraries are described in Section 6.2.

All executables use Python library functions either from the publicly available numpy, scipy and matplotlib libraries or the PROCESS Python libraries documented in Section 6.2. To use the PROCESS Python libraries you need to make sure their directory is in your Python path. Use the commands given in Section 4.1 to do this.

All Python code has been written for Python 3.

6.1 Executables

All executables can be run by using any of the following commands:

```
python executable_name.py
python3 executable_name.py
executable_name.py
```

and they typically have a short description of their usage when putting -h or --help as arguments:

```
executable_name.py -h
```

Some executables come with a configuration file that typically follows the naming convention executable_name.conf. To run the executable please copy the config file into your own work directory. Do **NOT** try to edit the config file in the PROCESS directory.

6.1.1 Turn output into input (write_new_in_dat.py)

This program modifies a given IN.DAT file such that the specified initial values of all the iteration variables are given by their values in OUT.DAT.

Input: IN.DAT, OUT.DAT

Output: new_IN.DAT

6.1.2 Randomly vary the starting point (run_process.py)

This program runs PROCESS many times, randomly varying the initial values of the iteration variables until a feasible solution is found. Stops when a feasible solution is found. If in the course of a scan some scan points result in feasible solutions and some do not, run_process.py will stop if and only if the number of unfeasible scan points is less than or equal to the parameter NO_ALLOWED_UNFEASIBLE.

Input: run_process.conf (optional), IN.DAT

Output: A directory is created for each run. containing all the standard PROCESS output, process.log (log file), and README.txt (contains comments from config file)

Configuration Options: The configuration file run_process.conf has the following style:

```
* This is a comment in the config file!

* Path to working directory in which PROCESS is run.
WDIR = Run1
* original IN.DAT name
ORIGINAL_IN_DAT = demo1a_10_sep_13.IN.DAT
* PATH to PROCESS binary
PROCESS = ~PROCESS/master/process
* ONE line comment to be put into README.txt
COMMENT = This is a test DEMO run! ;-)
* Maximum number of PROCESS runs
NITER = 5
* integer seed for random number generator; use None for random seed
SEED = 2
* factor within which the iteration variables are changed
FACTOR = 1.5
* Number of allowed unfeasible points that do not trigger rerunning.
NO_ALLOWED_UNFEASIBLE = 0
* include a summary file with the iteration variables at each stage.
INCLUDE_ITERVAR_DIFF = True
* add iteration variables - comma separated
ADD_IXC = 99, 77
* remove iteration variables - comma separated
DEL_IXC =
* add constraint equations  - comma separated
ADD_ICC = 57,
* remove constraint equations - comma separated
DEL_ICC =
* set any variable to a new value
```

```
* the variable does not have to exist in IN.DAT
VAR_TFTORT = 1.9
VAR_EPSVMC = 1e-4
* remove variables
DEL_VAR_IITER
```

A configuration file with an alternative name can be specified using the optional argument

```
run_process.py -f CONFIGFILE
```

6.1.3 List PROCESS runs with comments (build_index.py)

Creates an index of all PROCESS run comments, after they have been created by run_process in a series of subfolders.

Input: None

Output: Index.txt

Configuration Options: Optional arguments are:

```
# change the name of the file containing the folder description
build_index.py -r README.txt
# append the results to Index.txt instead of creating a new file
build_index.py -m a
# change the name of the subfolder Base - default=Run
build_index.py -b Base
# give a list of subfolder suffixes - default=all
build_index.py -s 1-4,6,8,9-12
# increase verbosity
build_index.py -v
```

An example Index.txt file might look like this

```
Run1:
 Original run

Run2:
 Changed the no. TF coils
...
```

6.1.4 test_process.py

This program has a similar structure to the `run_process.py` program, but varies the iteration variable start parameters for as many iterations as requested by the configuration file. It outputs a summary of the final iteration parameter values and figure of merit values for testing the accuracy of the optimisation solver in PROCESS.

Input: `test_process.conf`, an `IN.DAT` file as specified in the config file

Output: All the standard PROCESS output, `process.log`, `README.txt`, `time.info` (stores the run time of actual PROCESS iterations), `SolverTest.out`

The `SolverTest.out` file contains a table of the `ifail` values (see Table A.1), the figure of merit, the square root of the sum of the squares of the individual constraints as well as the initial and final values for the iteration variables and the individual constraint residuals. The value of Q, i.e. the ratio of fusion power to injected power, is also included in the SolverTest.out file. All values can be used to diagnose the performance of the optimisation solver.

Configuration Options: The configuration file `test_process.conf` has the following style:

```
* No iterations
NITER = 1000

* Working directory: Subdirectory in which to copy IN.DAT and test_process.conf
WDIR=Run1/

* original IN.DAT name (should not be called IN.DAT!)
ORIGINAL_IN_DAT = minimal_demo2_nosweep.IN.DAT

* sets flag of same name in IN.DAT:
*     None - keeps original value
*     -1   - Non-optimisation only
*      0   - one non-optimisation step followed by optimised iteration
*      1   - optimisation only
IOPTIMZ = 1

* sets the error tolerance for VMCON
*     None - keeps the original value (IN.DAT or default)
EPSVMC = None

* sets the step length for the finite difference derivatives
*     None - keeps the original value (IN.DAT or default)
EPSFCN = None


*sets the figure of merit
*positive value - minimise, negative value - maximise
```

```
*     None  - keeps the original value
*     1     - plasma major radius
*     6     - cost of electricity
MINMAX = None

* integer seed for random number generator; use None for random seed
SEED = 2

* factor within which the iteration variables are changed
FACTOR = 1.1

* PATH to PROCESS binary
PROCESS=process.exe
```

A configuration file with an alternative name can be specified using the optional argument

```
test_process.py -f CONFIGFILE
```

6.1.5 Output plotting: create data file (make_plot_dat.py)

Creates a `PLOT.DAT`-type file from `MFILE.DAT`. This is required by `plot_sweep.py`.

Input: `make_plot_dat.conf`, `MFILE.DAT`

Output: `make_plot_dat.out`

Configuration Options: Optional arguments are:

```
# new variables for output
make_plot_dat.py -p rmajor
# writes make_plot_dat.out in columns
make_plot_dat.py --columns
# resets make_plot_dat.conf to PLOT.DAT layout
make_plot_dat.py --reset-config
# file to read as input
make_plot_dat.py -f MFILE.DAT
# run with default parameters
make_plot_dat.py --defaults
```

An example version of `make_plot_dat.conf` might look like this:

```
# make_plot_dat.out config file.
rmajor
aspect
```

```
rminor
bt
powfmw
pnetelmw
te
pdivt
strtf1
strtf2
```

6.1.6 Create a two-page summary (plot_proc.py)

A utility to produce a two-page summary of the output, including the major parameters, poloidal and toroidal cross-sections, and temperature and density profiles.

Input: `MFILE.DAT`

Output: `proc_plot_out.pdf` (or as specified by user)

Configuration Options: Optional arguments are:

```
# change the input file name
python plot_proc.py -f MFILE.DAT
# change the output file name
python plot_proc.py -o out.pdf
# show the plot as well as saving the figure
python plot_proc.py -s
```

6.1.7 output_data.py

A utility to output a set of data very similar to **plot_proc.py**, but to a comma-delimited format for inclusion in spreadsheets. Not recommended - it's best to use PLOT.DAT instead, as this is always generated by PROCESS, and can be easily loaded into a spreadsheet.

Input: `MFILE.DAT`(or as specified by user)

Output: `process\_summary.txt` (or as specified by user)

Configuration Options: Optional arguments are:

```
# change the input file name
python output_data.py -f MFILE.DAT
# change the output file name
python output_data.py -o out.txt
```

6.1.8 plot_sweep.py

This utility plots normalised values from PLOT.DAT and allows comparisons of changes in values from a sweep compared to the first point in the sweep. It is now deprecated due to the existence of more flexible sweep-generating and output-handling utilities.

Input: PLOT.DAT as output by make_plot_dat.py

Output: PLOT.DAT.eps (default or as specified by user)

Configuration Options: Optional arguments are:

```
# creates PLOT.DAT.eps with R0, IP, beta
python plot_sweep.py -g 11 13 18
# creates demo1.png with Te, n
python plot_sweep.py -o demo1.png 21 22
```

6.1.9 Plot scan results (plot_mfile_sweep.py)

This utility plots normalised values of the iteration variables output by a parameter scan. Zero indicates an iteration variable at its lower bound and 1 an iteration variable at its upper bound.

Input: MFILE.DAT

Output: sweep_fig.pdf (default or as specified by user)

Optional arguments are:

```
# creates sweep_fig.pdf with R0, te, aspect (same variable names as in MFILE.DAT)
python plot_mfile_sweep.py -p rmajor te aspect
# creates demo1.png with Te, n
python plot_mfile_sweep.py -o demo1.png -p te dene
# creates a sweep_fig.pdf with R0, aspect with a different MFILE.DAT
python plot_mfile_sweep.py -f diff_mfile.dat -p rmajor aspect
# Show plot to screen instead of saving with R0 and aspect
python plot_mfile_sweep.py -p rmajor aspect --show

Use -h or --help for help
```

6.1.10 Plot iteration variables and constraint residuals (diagnose_process.py)

This utility aids the user to interpret PROCESS runs that do not find a feasible solution (unless PROCESS has terminated prematurely). It reads the MFILE.DAT and plots the normalised iteration variables, i.e. the iteration variable values normalised to their bounds such that 0 indicates an iteration variable at its lower bound and 1 an iteration variable at its upper bound. Furthermore, it shows the normalised constraint residuals.

Input: MFILE.DAT

Output: Displays plots on screen, still need to be saved by the user! (Remember to use -Y or -X, if sshing into a remote machine!)

Optional arguments are:

```
# allows to specify another location/name for the MFILE
python diagnose_process.py -f MFILE.DAT

Use -h or --help for help
```

6.1.11 fit_profile.py

This is a Python tool to fit a general temperature or density profile as given by the pedestalised profile parametrisation (`ipedestal` =1) to an ascii table. It is using a least squares method and is fitting the position of the pedestal as well as the peaking factors. Optional arguments are

```
-h, --help            show this help message and exit
-f FILENAME, --filename FILENAME
                      ascii file containing data in columns, default =
                      profile.txt
-r RHO, --rho RHO     column of the normalised radius rho=r/a, default = 0
-n DENSITY, --density DENSITY
                      column of the density profile, default = 1
-t TEMPERATURE, --temperature TEMPERATURE
                      column of the temperature profile, default = 2
-rn RHOPEDN, --rhopedn RHOPEDN
                      user defined initial guess of the density pedestal
                      position, if outside [0,1] starts at 0.9, default =
                      0.9
-rt RHOPEDT, --rhopedt RHOPEDT
                      user defined initial guess of the temperature pedestal
                      position, if outside [0,1], starts at 0.9, default =
                      0.9
```

If the column of the density or temperature data does not exist, it is ignored. A warning is issued.

6.1.12 Step from one model to another (a_to_b.py)

When attempting to model a reactor very different from those in previous studies, it can be difficult to find a feasible solution. This utility takes an initial `IN.DAT` (`A.DAT`) that is known to run successfully, and a target `IN.DAT` (`B.DAT`) that is substantially different. The difference is broken into small steps, and `PROCESS` runs repeatedly, stepping from the initial input file to the target input file. After each step, the output values of the iteration variables are used as the input starting values for the next step.

Input: `a_to_b.conf`, `A.DAT` and its corresponding `MFILE.DAT`, `B.DAT`. (These names can be changed by the user.)

Output

When the program finishes, the .DAT files from the last run of PROCESS can be found in the specified working directory.

If option keep_output = True, then IN.DAT, OUT.DAT, MFILE.DAT and logged PROCESS output of each step are stored. Files are prefaced with their step number eg. 003.IN.DAT and copied to the specified output directory.

Configuration Options: The configuration file a_to_b.conf has the following style:

```
*Comment line

*Working directory to store temporary files, default = wdir
wdir = wdir

*Switch to keep .DAT files for every step, default = True
keep_output = True

*Directory for output if keep_output = True, default = steps
outdir = steps

*IN.DAT file for A, default = A.DAT
a_filename = A.DAT

*IN.DAT file for B, default = B.DAT
b_filename = B.DAT

*Path to process binary
*path_to_process = /home/PROCESS/master/process
path_to_process = /home/PROCESS/master/process

*Number of iterations of vary_iteration_variables to run, default = 20
vary_niter = 20

*Number of steps to go from A to B, default = 10
nsteps = 10

*Factor to vary iteration variables within, default = 1.2
factor = 1.2

*Gap between upper and lower bounds to narrow to, default = 1.001
bound_gap = 1.001
```

6.1.13 N-Dimensional Scanner Utility

This suite of Python utilities allows the user to conduct systematic, multi-dimensional parameter studies with `PROCESS`. It systematically varies a set of N user defined parameters within predefined bounds. The final results can be evaluated using the corresponding visualisation tool and/or saved in standard NetCDF format for further analysis.

The suite contains the following executables

- `ndscan.py` - executes the Nd-scan as specified in the configuration file.
- `ndscan_package_only.py` - creates a NetCDF output file from a previous Nd-scan run.
- `ndscan_and_package.py` - both executes the Nd-scan and creates the NetCDF output file.
- `ndscan_visualisation.py` - visualises the NetCDF output.

Input: `ndscan.json`, `IN.DAT`

Output: All MFILES in subdirectory `MFILES`, packaged NetCDF output file as named in configuration file (default "NdscanOutput.nc").

When running any of the ndscan tools, optional arguments are:

```
#to specify another location/name for the configfile
ndscan.py -f CONFIGFILE

Use -h or --help for help
```

For the visualisation tool the corresponding NetCDF input file can also be specified with `-f`. Per default "NdscanOutput.nc" is used.

Configuration Options: The configuration file `ndscan.json` uses the JSON format[1] and has the following style

```
{
    "axes": [
{
            "lowerbound": 7.5,
            "steps": 16,
            "upperbound": 9.0,
            "varname": "rmajor"
        },
        {
            "lowerbound": 5.5,
            "steps": 16,
            "upperbound": 7.0,
```

[1] www.json.org

```
            "varname": "bt"
        }
    ],
    "_comment": [
        "This field helps to describe the config file for users reading",
        "Anything you write in here will be ignored by the code",
        "Each axis has these configuration parameters available:",
        "varname",
        "lowerbound",
        "upperbound",
        "'steps': number of evaluations"
    ],
    "optionals": {
        "remove_scanvars_from_ixc": true,
        "smooth_itervars": true
    },
    "description": "Description of the goals of this specific run",
    "title": "NdscanOutput",
    "author": "Me",
    "output_vars": [
        "beta",
        "pheat",
        "powfmw",
        "pradmw",
        "powerht",
        "cirpowfr",
        "te",
        "hfact",
        "dnelimt",
        "dene",
        "rmajor",
        "bt",
        "pnetelmw",
        "coe",
        "fwbllife",
        "capcost",
        "palpmw",
        "wallmw",
        "taueff"
    ]
}
```

The only required input parameter in the configuration file are the scan axes, out of which at least one has to be specified. For each axis a `varname`, a `lowerbound`, an `upperbound` and the number of `steps` > 1 have to be specified. All other parameters in the configuration file are optional. The parameters relevant for running the N-dimensional scan are:

`_comment` Anything in the comment section (like all other undefined sections) is for the user only and

will be ignored by the program.

`optionals:remove_scanvars_from_ixc` Removes all scanning variables from the iteration variables of the IN.DAT file (default=True).

`optionals:smooth_itervars` Ensures that each next point starts from the last successful run. This increases the run time, but improves convergence and reduces errors.

The parameters only relevant to the creation of the summary NetCDF file are:

`author` The author will be copied into the NetCDF file.

`description` The description will be copied into the NetCDF file.

`title` Name of the output NetCDF file (default `NdscanOutput`) that is also copied into the title of the NetCDF file.

`output_vars` The variables that will be extracted from the MFILEs and stored in the NetCDF file. (Only needed when creating the NetCDF output file.)

Additional parameters can be specified as in the `config` section for the `evaluate_uncertainties.py` tool, see section 6.1.14.1.

The resulting NetCDF file can be visualised using the `ndscan_visualisation.py` tool. It has an interactive menu and is fairly self-explanatory.

6.1.14 Uncertainty Tools

In this section, we explain the usage of the `PROCESS` tools to both evaluate the uncertainties of a design point as well as display them using a simple plotting facility.

Note that the uncertainty evaluation tool has a significantly longer run time than typical evaluations of `PROCESS` design points and therefore should only be used once a suitable design point has been found. As only user selected output data is kept, the user is recommended to put careful thought into the list of needed output variables.

6.1.14.1 evaluate_uncertainties.py

This program evaluates the uncertainties of a single `PROCESS` design point by use of a Monte Carlo method as described in [83]. It takes a set of uncertain parameters as input, each of which can have either a Gaussian or a flat ('top-hat') probability distribution. These are specified together with optional details about the `PROCESS` run in a configuration file. Additionally, an `IN.DAT` file describing the relevant design point needs to be present. (If necessary this can be created from an `MFILE.DAT` by using the `write_new_indat.py` tool.)

When running the `evaluate_uncertainties.py` tool, optional arguments are:

```
#to specify another location/name for the configfile
evaluate_uncertainties.py -f CONFIGFILE

Use -h or --help for help
```

Input: `evaluate_uncertainties.json`,
`IN.DAT` (or an alternative input file as specified in the config file)

Output:
`uncertainties.nc`. This file (NetCDF format) can be visualised using the `display_uncertainties.py` tool.
`Readme.txt`,
`process.log`,
`PROCESS` output from the last run.

The configuration file `evaluate_uncertainties.json` uses the JSON format[2], and has the following style

```
{
"_description": "Config file for uncertainties evaluation",
"_author": "Hanni Lux",

"config": {
  "runtitle": "testrun for uncertainty tool on DEMO2",
  "IN.DAT_path": "IN.DAT_demo2",
  "process_bin": "~PROCESS/master/process.exe",
  "working_directory": "Run1",
  "pseudorandom_seed": 2
  },
"uncertainties": [
                {
                     "Varname":"flhthresh",
                     "Errortype":"Gaussian",
                     "Mean":1.0,
                     "Std":0.05
                },
                {
                     "Varname":"coreradius",
                     "Errortype":"Uniform",
                     "Lowerbound":0.6,
                     "Upperbound":0.9
                },
                {
                     "Varname":"etanbi",
                     "Errortype":"Relative",
                     "Mean":0.3,
                     "Percentage":10.0
                },
                {
                     "Varname":"boundu(9)",
                     "Errortype":"LowerHalfGaussian",
```

[2] www.json.org

```
                    "Mean":1.2,
                    "Std":0.1
               },
               {
                    "Varname":"boundl(103)",
                    "Errortype":"UpperHalfGaussian",
                    "Mean":1.0,
                    "Std":0.25
               }
      ],
     "output_vars": [ "rmajor", "dene", "te", "bt"],
     "no_samples": 1000
}
```

By convention, we have designated metadata about the PROCESS runs as having a preceding underscore to distinguish these values from the other configuration data used directly by the tools or PROCESS itself. Furthermore, all the optional attributes that can be changed when running PROCESS from most Python utilities like e.g. run_process.py can be specified in the "config" section. All these values have default values and do not need to be set.

runtitle is a one line description of the purpose of the run to be saved in Readme.txt in the working directory as well as the runtitle parameter in the OUT.DAT and MFILE.DAT files. Per default it is empty.

IN.DAT_path is the name/path of the IN.DAT file describing the design point. If not specified it is assumed to be IN.DAT.

process_bin is the process binary that should be used. The default assumes that the user works on the CCFE Fusion Linux machines and has executed the module commands for PROCESS as described in 4.1. Then either the master or development branch of process is being used depending on which module has been loaded.

working_directory represents the working directory, in which PROCESS will be executed, in case this is supposed to be different to the current directory which can be helpful when executing several runs with slightly different setups.

pseudorandom_seed is the value of the seed for the random number generator. It can be any integer value. If it is not specified, its default value is taken from the system clock.

Other parameters that can be specified in the config section are Niter and factor. Both do not typically need to be changed by the user. Niter is the maximum number of retries that the tool will attempt, if PROCESS fails to find a feasible solution. This means that the tool varies the start values of the iteration variables within a factor given by factor of the original values as this does not change the physical meaning of the input file, but can help the solver to find a better starting point for its iteration. Their default values are Niter=10 and factor=1.5.

Any uncertain parameters should be specified in the "uncertainties" section. Each parameter is specified in its own sub dictionary as shown in the example. For each, the Varname and Errortype need to be specified as well as the Mean and standard deviation Std for Gaussian type errors as well as Lowerbound and Upperbound for Uniform or Mean and a Percentage for Relative errors. Apart from

a standard Gaussian distribution, also a lower and an upper half Gaussian distribution are available that have a sharp cut off at the mean. Please note, that *all distributions are being cut off at the boundaries for the input values for* `PROCESS!` At least one uncertain parameter has to be specified for the program to run and technically there is no upper limit as to how many uncertain parameters can be used. However, for large numbers of uncertain parameters it is recommended to increase the number of sampling points.

There are a number of other parameters in the configuration file that can be specified:

`output_vars` is a list of strings of output variable names in the `MFILE.DAT`. These are the variables saved. This list is empty by default and it is therefore crucial for the user to specify the variables of interest because otherwise the tool will not run.

`no_samples` sets the number of sample points in the Monte Carlo method. It is by default set to its recommended minimum value of 1000, but the user should contemplate higher values especially if a large number of uncertain parameters is involved.

Two parameters that can be further set in the config file (but are not recommended to be changed) are the number of scan points `no_scans` which is by default 5 and the number of allowed unfeasible points in a scan `no_allowed_unfeasible` which is 2 as recommended in [83].

As the distributions of the uncertainties do not have to be represented by a simple Gaussian, reducing the output to two simple numbers like a mean and a standard deviation is not typically possible. Therefore, we have decided to keep all sampled points in the output files. However, to reduce the amount of data we have decided to only store the user specified parameters in the form of a NetCDF binary file. Given that a scan is performed at each sample point, only the last of these scan points is ever kept for evaluation. (There is an option for developers to keep all the data for debugging purposes. However, this should typically not be used in production runs.) These files can be visualised using the `display_uncertainties.py` tool.

6.1.14.2 display_uncertainties.py

This is a utility to display the output file `uncertainties.nc` created by the `evaluate_uncertainties.py` tool described above.

By default, if run in the working directory of an uncertainty evaluation, it creates a scatter plot of each user defined output parameter against the next parameter in the list. It also shows the 1D histograms of each parameter distribution. If two specific variables are given as arguments, the tool plots only these two against each other.

Input: `uncertainties.nc`

Output: Uncertainties_varname1_varname2.pdf

Usage:

```
display_uncertainties.py [-h] [-f FILENAME] [-e END] [v [v ...]]

Program to display uncertainties of a given PROCESS design point.

positional arguments:
  v              list of variables to be plotted; default = all
```

```
optional arguments:
  -h, --help     show this help message and exit
  -f FILENAME, --filename FILENAME
                 uncertainties data file, default = uncertainties.nc
  -e END, --end END     file format default = .pdf
```

6.1.15 create_dicts.py

This automatically generates the `process_dicts.py` file used by `PROCESS`utility programs. It does this by scanning the Fortran source code. The standard output should be redirected, using

```
create_dicts.py > process_dicts.py
```

6.1.16 Batch Jobs

As `PROCESS` typically runs very fast and does not produce much data output, it is not typically necessary to submit `PROCESS` runs or any of the python executables as a batch job to the fusion linux machines. However, the `evaluate_uncertainties.py` tool is one example of a python tool for `PROCESS` that does run for a long time and does create a lots of output. As the CPU time limit for any non-batch jobs on the fuslw machines is 30 Minutes, any decently sampled `evaluate_uncertainties.py` run will need to be submitted as a batch job. (Please note, that if you have forgotten to submit your job as a batch job, your job will be terminated after 30 CPU minutes, but as the output is written to file continuously, you should not loose any of the output that has been produced until then.)

To submit a batch job, first create a file called e.g. myjob.cmd. It should contain the following content

```
# @ executable = evaluate_uncertainties.py
# @ arguments
# @ input = /dev/null
# @ output = /ABSOLUTE_PATH_TO_WORK_DIR/ll.out
# @ error = /ABSOLUTE_PATH_TO_WORK_DIR/ll.err
# @ initialdir = /ABSOLUTE_PATH_TO_WORK_DIR/
# @ notify_user = USERNAME
# @ notification = complete
# @ queue
module use /home/PROCESS/modules
module swap python
module load process/master
evaluate_uncertainties.py
```

Once you have created the file you can submit a batch job by typing

```
llsubmit myjob.cmd
```

While your job is running you can keep track of its progress by typing `llq` or `xloadl`. More information and help with troubleshooting can be found under `http://fusweb1.fusion.ccfe.ac.uk/computing/funfaq/ll/`.

As the uncertainties.nc output file can get quite large, it might be indicated to write the output to the /scratch or /tmp directories as they have faster I/O. Please remember to copy your results into your home directory afterwards, as these directories are not backed up and will be frequently cleaned.

6.1.17 mfile_comparison.py

Tool for comparing two MFILEs and outputting significant differences in numerical values.

Arguments
`-f` Files to compare
`-s` Save output to file called comp.txt
`--acc` Percentage difference threshold for reporting
`--verbose` Additional output

6.1.18 test_suite.py

The PROCESS test suite allows PROCESS developers to quickly test new modifications to PROCESS using a defined library of reference cases. The test suite is bundled with PROCESS and is a single Python script (**test_suite.py**) with a number of options.

The test suite will provide the following output

- Summary to terminal and file (**summary.log**)
- PROCESS terminal output log to file for each test case (**run.log**)
- PROCESS error log to terminal and to file if errors for each test case (**error.log**)
- New MFILE.DATs and OUT.DATs for each test case (**new.MFILE.DAT** and **new.OUT.DAT**)

6.1.18.1 Folder Structure

The PROCESS folder structure is shown below. The test suite folder (**test_suite**) is in the main directory with the FORTRAN files. Inside the test suite folder there is the main code (**test_suite.py**) as well as the folders containing the reference cases (**test_files**). The figure below shows the folder structure for the test_suite.

6.1.18.2 Adding a reference case

To add a reference case if you have a local PROCESS repository:

1. Have an IN.DAT that works with the current version of PROCESS
2. Run PROCESS to create an OUT.DAT and MFILE.DAT
3. Create a folder in the location **/my_develop/test_suite/test_files/[test_name]** with a suitable name for the test case (if your local PROCESS folder is `my_develop`).
4. Copy your IN.DAT, OUT.DAT and MFILE.DAT into this folder

5. Copy IN.DAT as **ref.IN.DAT**
6. Rename OUT.DAT as **ref.OUT.DAT**
7. Rename MFILE.DAT as **ref.MFILE.DAT**
8. `cd ../..` to return to test_suite folder
9. `test_suite.py` to run the test suite to check it works
10. Commit to Git locally and push to the central repository (see instructions in PROCESS manual)

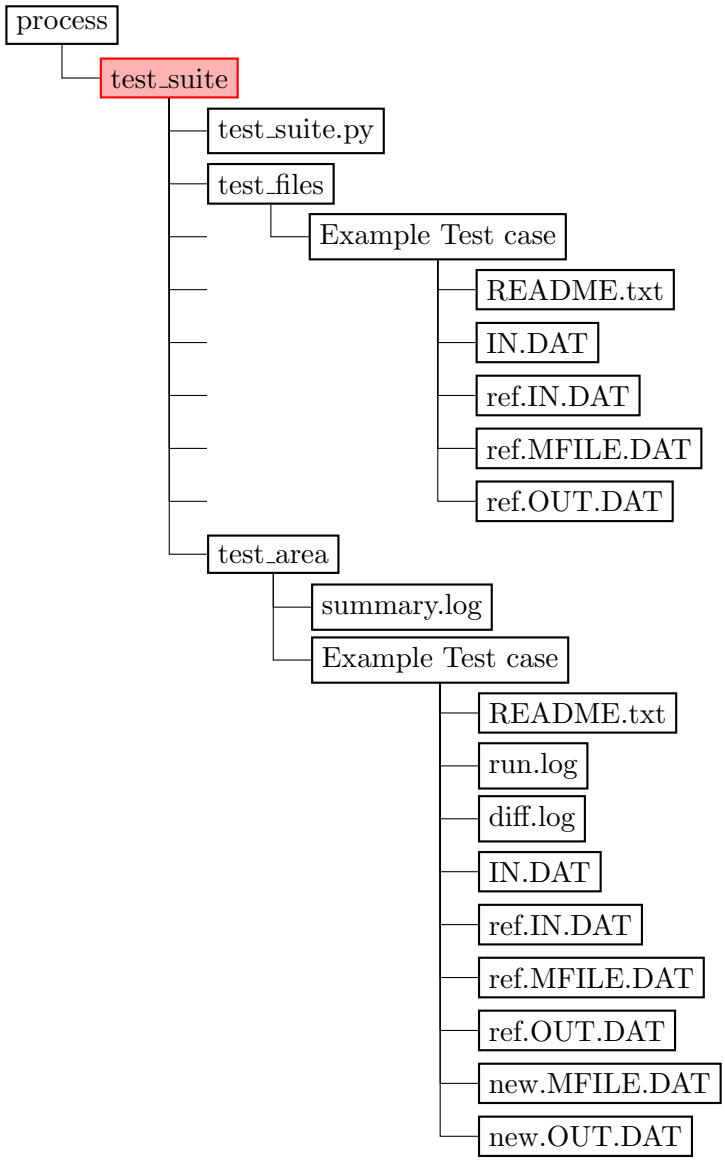


Figure 6.1: PROCESS Test suite folder structure after a test run. The test_area folder is where the output of the test run is stored. Each test case has a README file which outlines the reasoning for the test.

6.1.18.3 Running the Test Suite

To run the test suite the user should go to the folder **/process/test_suite/** and then run the Python file **test_suite.py**. The test suite Python script has the following optional arguments.

```
 python test_suite.py [options]

 -h - -help         show usage

 -s --save          save test output to folder with PROCESS revision
number in it(e.g. test_r383)

 -d --diff [val]    set allowed difference between reference case and
new output in percentage terms.

 -r --ref           choose reference folder to use for the test cases
                    default is "test_files"

 --debug            run reference cases prefixed with "error_" for
                    testing of the error handling in the test suite

 Examples

    python test_suite.py -d 10 --save

    python test_suite.py -d 1
```

6.1.18.4 Test Suite Output Formatting

summary.log

The summary.log file mirrors what was displayed to the terminal during a test suite run. It will look something like the following.

```
PROCESS Test Suite

Date: 2015-12-03
Diff set to: 5.0%

PROCESS Test Cases

Test ==>  DEMO1_a31_06_2015            DIFF(6)
Test ==>  costs_paper                  OK
Test ==>  test 3                       ERROR
Test ==>  test 4                       OK

PROCESS version r[version] test run complete
```

diff.log

This file will contain the differences between the reference case and the new run for a given test. The file will look like the example below.

```
PROCESS Test Suite

Test Case: [test_name]
Difference value: [diff]

Differences above allowed value:

    var | ref | new | %
    a     10    15    50
    b     10    9     10
    ...   ...   ...   ...

Variables in ref NOT IN new:

    var 1
    var 2
    ...

Variables in new NOT IN ref:

    var 1
    var 2
    ...
```

run.log

Run.log will take the output to the terminal for each PROCESS test case and dump it to a file in the test folder in **/process/test_suite/test_area/[test_name]/**. If there is an error while running PROCESS this will be highlighted in **summary.log** and then the user can inspect the output in run.log

new.MFILE.DAT

This is the MFILE.DAT the test suite created when running a given test case. After running the test suite will move this file to the folder **/process/test_suite/test_area/[test_name]/**.

new.OUT.DAT

This is the OUT.DAT the test suite created when running a given test case. After running the test suite will move this file to the folder **/process/test_suite/test_area/[test_name]/**.

6.2 Python Libraries

All library modules and functions are documented using docstrings. These can be accessed by reading the code directly or via the `help()` function in Python.

6.2.1 in_dat.py

A set of Python classes to read, modify and write an `IN.DAT` file.

`INVariable(name, value, comment="")` Initialises an `IN.DAT` variable class which requires a name and a value.

`INModule(name)` Initialises an `IN.DAT` module class which requires a name. This class stores information for an `IN.DAT` file which has modules separated with lines with $MODULE_NAME and $END.

`INModule.add_variable(var)` Adds an `INVariable` object to the `INModule` class.

`INModule.remove_variable(variable_name)` Removes an `INVariable` object from the `INModule` class.

`INModule.add_line(line)` Adds a line from the `IN.DAT` that isn't a variable line (e.g. a comment) to the `INModule` class.

`INModule.get_var(var_name)` Returns an `INVariable` object from the `INModule` class.

`INModule.add_constraint_eqn(eqn_number)` Adds constraint equation `eqn_number` to the list of constraint equations `InVariable` class if the equation is not already in the list.

`INModule.remove_constraint_eqn(eqn_number)` Removes constraint equation `eqn_number` from the list of constraint equations `InVariable` class if the equation is already in the list.

`INModule.add_iteration_variable(var_number)` Adds iteration variable `var_number` to the list of iteration variables `InVariable` class if the variable is not already in the list.

`INModule.remove_iteration_variable(var_number)` Removes iteration variable `var_number` to the list of iteration variables `InVariable` class if the variable is already in the list.

`INDATClassic(filename="IN.DAT")` Initialises an `IN.DAT` class which can be given a different filename. This class is used for an `IN.DAT` with a module structure.

`INDATClassic.read_in_dat()` Reads an `IN.DAT` file with modular structure.

`INDATClassic.write_in_dat(filename="new_IN.DAT")` Writes a new `IN.DAT` with modular structure.

`INDATNew.read_in_dat()` Reads an `IN.DAT` file without modular structure.

`INDATNew.write_in_dat(filename="new_IN.DAT")` Writes a new `IN.DAT` without modular structure.

`INDATNew.add_variable(var)` Adds an `INVariable` object to the `INDATNew` class.

`INDATNew.remove_variable(var_name)` Removes an `INVariable` object from the `INDATNew` class.

`INDATNew.add_constraint_eqn(eqn_number)` Adds constraint equation `eqn_number` to the list of constraint equations `InVariable` class if the equation is not already in the list.

`INDATNew.remove_constraint_eqn(eqn_number)` Removes constraint equation `eqn_number` from the list of constraint equations `InVariable` class if the equation is already in the list.

`INDATNew.add_iteration_variable(var_number)` Adds iteration variable `var_number` to the list of iteration variables `InVariable` class if the variable is not already in the list.

`INDATNew.remove_iteration_variable(var_number)` Removes iteration variable `var_number` to the list of iteration variables `InVariable` class if the variable is already in the list.

`clear_lines(lines)` Removes comment only lines and replaces multiple empty lines with a single empty line.

`variable_type(var_name, var_value)` Checks the type of an `IN.DAT` variable using `DICT_VAR_TYPE`

`fortran_python_scientific(var_value)` Changes from FORTRAN double precision notation `D` to Python's `e` notation.

6.2.2 mfile.py

A set of Python classes to read and extract data from `MFILE.DAT`.

`MFileVariable(var_name, var_description)` Object to contain information for a single `MFILE.DAT` variable.

`MFileVariable.set_scan(scan_number, scan_value)` Sets the variable value for scan number `scan_number`

`MFileVariable.get_scan(scan_number)` Returns the variable value for scan number `scan_number`

`MFileVariable.get_scans()` Returns the variable value for all scans.

`MFile(filename="MFILE.DAT")` Object to contain information for all variables in an `MFILE.DAT` for all scans.

`MFile.search_keys(variable)` Search for an MFILE variable in the data dictionary.

`MFile.search_des(description)` Search for an MFILE description in the data dictionary.

`MFile.make_plot_dat(custom_keys, filename="make_plot_dat.out", file_format="row")` Create a `PLOT.DAT` equivalent for the variables in `custom_keys` in either row or column format.

`MFile.get_num_scans()` Returns the number of scans in the `MFILE.DAT`

`read_mplot_conf(filename="make_plot_dat.conf")` Reads the config file `make_plot_dat.conf` and fills the list `custom_keys` with these variables.

`write_mplot_conf(filename="make_plot_dat.conf")` Writes a new `make_plot_dat.conf` adding any additional variables that the user `gave make_plot_dat.py` at runtime.

6.2.3 process_funcs.py

This library contains a collection of functions used by various `PROCESS` utilities.

`get_neqns_itervars(wdir='.')` Returns the number of equations and a list of variable names of all iteration variables.

`update_ixc_bounds(wdir='.')` Updates the lower and upper bounds in `DICT_IXC_BOUNDS` from `IN.DAT`.

`get_variable_range(itervars, factor, wdir='.')` Returns the lower and upper bounds of the variable range for each iteration variable.

`itervars`: string list of all iteration variable names

`factor`: defines the variation range for non-f-values by setting them to value * factor and value / factor respectively while taking their `PROCESS` bounds into account.

For f-values the allowed range is equal to their `PROCESS` bounds.

`check_logfile(logfile='process.log')` Checks the log file of the `PROCESS` output. Stops if an error occurred that needs to be fixed before rerunning.

`process_stopped(logfile='process.log')` Checks the `PROCESS` logfile whether it has prematurely stopped.

`process_warnings(logfile='process.log')` Checks the `PROCESS` logfile whether any warnings have occurred.

`mfile_exists()` Checks whether `MFILE.DAT` exists.

`no_unfeasible_mfile(wdir='.')` Returns the number of unfeasible points in a scan in `MFILE.DAT`.

`no_unfeasible_outdat(wdir='.')` Returns the number of unfeasible points in a scan in `OUT.DAT`.

`vary_iteration_variables(itervars, lbs, ubs)` Changes the iteration variables in `IN.DAT` within given bounds.

`itervars`: string list of all iteration variable names

`lbs`: float list of lower bounds for variables

`ubs`: float list of upper bounds for variables

`get_solution_from_mfile(neqns, nvars, wdir='.')` Returns:-

- `ifail`: error value of `PROCESS`
- the objective functions
- the square root of the sum of the squares of the constraints
- a list of the final iteration variable values
- a list of the final constraint residue values
- If the run was a scan, the values of the last scan point will be returned.

`get_solution_from_outdat(neqns, nvars)` Returns:-

- `ifail`: error value of `PROCESS`
- the objective functions
- the square root of the sum of the squares of the constraints
- a list of the final iteration variable values
- a list of the final constraint residue values
- If the run was a scan, the values of the last scan point will be returned.

6.2.4 process_config.py

A collection of Python classes for configuration files used by various `PROCESS` utilities, e.g. `run_process.py` or `test_process.py`. It contains a base class `ProcessConfig` and two derived classes `RunProcessConfig` and `TestProcessConfig`.

`ProcessConfig()` Object that contains the configuration parameters for PROCESS runs.

`filename` : Configuration file name

`wdir` : Working directory

`or_in_dat` : Original `IN.DAT` file

`process` : `PROCESS` binary

`niter` : (Maximum) number of iterations

`u_seed` : User specified seed value for the random number generator

`factor` : Multiplication factor adjusting the range in which the original iteration variables should be varied

`comment` : Additional comment to be written into `README.txt`

`ProcessConfig.echo_base()` Echos the attributes of the base class to standard output.

`ProcessConfig.echo()` Echos the values of the current class to standard output.

`ProcessConfig.prepare_wdir()` Prepares the work directory for the run.

`ProcessConfig.create_readme(directory='.')` Creates a file called `README.txt` containing `ProcessConfig.comment`.

`ProcessConfig.modify_in_dat()` Modifies the original `IN.DAT` file.

`ProcessConfig.setup()` Sets up the program for running.

`ProcessConfig.run_process()` Runs `PROCESS` binary.

`ProcessConfig.get_comment()` Gets the comment line from the configuration file.

`ProcessConfig.get_attribute(attributename)` Gets a class attribute from the configuration file.

`ProcessConfig.set_base_attributes()` Sets the attributes of the base class.

`TestProcessConfig(filename='test_process.conf')` Object that contains the configuration parameter of the `test_process.py` program.

`ioptimz` : sets `ioptimz` (optimisation solver) in `IN.DAT`.

`epsvmc` : sets `epsvmc` (VMCON error tolerance) in `IN.DAT`.

`epsfcn` : sets `epsfcn` (finite diff. steplength) in `IN.DAT`.

`minmax` : sets `minmax` (figure of merit switch) in `IN.DAT`.

`TestProcessConfig.echo()` Echos the values of the current class to std out.

`TestProcessConfig.modify_in_dat()` Modifies `IN.DAT` using the configuration parameters.

`RunProcessConfig(filename='run_process.conf')` Configuration parameters of the `run_process.py` program.

`no_allowed_unfeasible` : The number of allowed unfeasible points in a sweep

`create_itervar_diff` : Boolean to indicate the creation of a summary file of the iteration variable values at each stage

`add_ixc` : List of iteration variables to be added to `IN.DAT`.

`del_ixc` : List of iteration variables to be deleted from `IN.DAT`.

`add_icc` : List of constrained equations to be added to `IN.DAT`.

`del_icc` : List of constrained equations to be deleted from `IN.DAT`.

`dictvar` : Dictionary mapping variable name to new value (replaces old or gets appended)

`del_var` : List of variables to be deleted from `IN.DAT`.

`RunProcessConfig.get_attribute_csv_list(attributename)` Get a class attribute list from the configuration file; expects comma separated values.

`RunProcessConfig.set_del_var()` Sets the `RunProcessConfig.del_var` attribute from the config file.

`RunProcessConfig.set_dictvar()` Sets the `RunProcessConfig.dictvar` attribute from config file.

`RunProcessConfig.echo()` Echos the values of the current class.

`RunProcessConfig.modify_in_dat()` Modifies `IN.DAT` using the configuration parameters.

`RunProcessConfig.modify_vars()` Modifies `IN.DAT` by adding, deleting and modifiying variables.

`RunProcessConfig.modify_ixc()` Modifies the array of iteration variables in `IN.DAT`.

`RunProcessConfig.modify_icc()` Modifies the array of constraint equations in `IN.DAT`.

6.2.5 process_dicts.py

A collection of dictionaries and lists used by various `PROCESS` utilities.

`IFAIL_SUCCESS` This is the `PROCESS` error code of a successful run.

`PARAMETER_DEFAULTS` Default values for making a `PLOT.DAT` file from `MFILE.DAT`.

`DICT_VAR_TYPE` Maps the `PROCESS` variable name to its value type. The value type can be one of `int_array`, `int_variable`, `real_array` or `real_variable`.

`DICT_IXC_SIMPLE` Maps the string number of the iteration variable to its variable name.

`DICT_IXC_FULL` Maps the string number of the iteration variable to a dictionary that contains the variable name under 'name', the default lower variable bound (float) under 'lb' and the default upper variable bound (float) under 'ub'.

`DICT_IXC_BOUNDS` Maps each iteration variable name to a dictionary that contains the default lower variable bound (float) under 'lb' and the default upper variable bound (float) under 'ub'.

`NON_F_VALUES` List of iteration variable names that start with an f, but are not f-values.

`DICT_NSWEEP2IXC` Maps the sweep variable number `nsweep` to the respective iteration variable number, if applicable.

`DICT_IX2NSWEEPC` Maps the iteration variable number to the respective sweep variable number `nsweep`, if applicable.

`DICT_TF_TYPE` Maps the `PROCESS` TF coil type number to its type.

`DICT_OPTIMISATION_VARS` Maps each figure of merit number to its description.

`DICT_IXC_DEFAULT` Maps each iteration variable name to its default value.

Add new stuff used by GUI etc.

6.2.6 a_to_b_config.py

To do...

6.2.7 proc_plot_func.py

A collection of functions and lists used by `plot_proc.py`.

`RADIAL_BUILD` A list of radial build variables.

`VERTICAL_BUILD` A list of vertical build variables.

`FILL_COLS` A list of plotting colours

For all of the functions below the arguments are:

`axis` : Matplotlib axis object to plot to

`mfile_data` : MFILE data object `MFile`

`scan` : Scan number to plot

`plot_plasma(axis, mfile_data,scan)` Function to plot plasma

`poloidal_cross_section(axis, mfile_data, scan)` Function to plot machine build

`plot_tf_coils(axis, mfile_data, scan)` Function to plot the TF coils

`plot_pf_coils(axis, mfile_data, scan)` Function to plot the PF coils

`plot_geometry_info(axis, mfile_data, scan)` Function to plot the geometry info block

`plot_physics_info(axis, mfile_data, scan)` Function to plot the physics info block

`plot_magnetics_info(axis, mfile_data, scan)` Function to plot the magnetics info block

`plot_power_info(axis, mfile_data, scan)` Function to plot the power info block

`plot_current_drive_info(axis, mfile_data, scan)` Function to plot the current drive info block

`plot_geometry_info(axis, mfile_data, scan)` Function to plot the geometry info block

6.2.8 diagnose_funcs.py

A collection of functions used by `diagnose_process.py`.

`plot_normalised_ixc(mfilename='MFILE.DAT')` Plots the normalised values of the iteration variables of a given `MFILE.DAT`.

`plot_normalised_icc_res(mfilename='MFILE.DAT')` Plots the normalised values of the costraint residuals of a given `MFILE.DAT`.

6.3 User Interface

The user interface is still being developed, but currently allows for viewing and editing of `IN.DAT` files in a web browser. It can be found in the `utilities/gui` directory. See 4.2 for details.

Chapter 7

Code Management Tools

This chapter will be of interest to people involved in the continuing maintenance of the `PROCESS` source code. As stated elsewhere, the source code is maintained by CCFE, and resides in a Git repository on the CCFE servers.

7.1 The Makefile

In addition to its normal role for compilation, the makefile (named `Makefile`) includes a number of utility functions that perform tasks such as automatic generation of the code documentation, and the creation of a tar file containing the entire source code, its documentation files, and the input and output files. This has proved to be of great benefit in keeping all of the data from a given run together for archival purposes.

7.1.1 Compilation

Compilation is trivially performed using the makefile. Currently, the available options are (type the following on the command line):

`make ARCH=FUN`	CCFE Fusion Unix Network (Intel Fortran ifort compiler)
`make ARCH=GFORT`	GNU Fortran compiler (gfortran; N.B. only versions 4.6.3 or above)
`make ARCH=JAC`	JET Analysis Cluster (pgf95 compiler)

The Intel Fortran compiler is the default option, so typing simply `make` will have the same effect as typing `make ARCH=FUN`.

The code is almost trivial to port to new architectures, by adding extra stanzas to the makefile as required.

To force a full recompilation, type `make clean`. N.B. This will remove (without prompting) all "backup" files (`*~`) as well as certain other files from the working directory.

Extra run-time diagnostics (array-bound checking, etc.) is turned on by default at present; the code is sufficiently quick to run that the performance penalty is barely noticeable. However, this can be turned off (beware... results can change!), by adding `DEBUG=NO` to the relevant command above, i.e. type `make ARCH=... DEBUG=NO`. N.B. there must be no spaces either side of the `=` characters in any of the above commands.

7.1.2 Archiving utilities

The makefile can be used in a number of ways to pack the various file sets together into a single compressed tar file, for ease of portability and archiving.

- `make tar`: Typing this command produces a file `process.tar.gz` that contains all of the source files, utility programs and documentation files necessary to run the program from scratch on a new machine or in a new directory. (Note that the input files `IN.DAT` and `device.dat` are not included.) This is useful for transferring new copies of source files, etc. into an existing directory already containing a previous `PROCESS` run, as the pre-existing customised input files will not be overwritten. To extract the individual files again, copy the file to the destination working directory and type `tar zxvf process.tar.gz`
- `make archive`: Typing this command produces a file `process_run.tar.gz` containing the working directory's input and output files (`IN.DAT`, `OUT.DAT`, `PLOT.DAT`, `MFILE.DAT` and `device.dat` (which must exist to avoid an error message; see Section B.0.1), together with all of the source files, utility programs and documentation files. These files together comprise the full set that define a given run, and so the file produced by this command is suitable for long-term storage for archival purposes. To extract the contents, type `tar zxvf process_run.tar.gz`

Note that each of the above commands will overwrite the given named tar file if one already exists in the working directory.

7.1.3 Code documentation

The makefile can also be used to produce source code documentation, as described in the next section.

7.2 Automatic Documentation

The `PROCESS` source code is self-documenting to a degree, using an included parser program (`autodoc`) to generate html files for each subprogram from specially-formatted comment lines within the code. It is the responsibility of the programmer to keep the `autodoc` comments within the source code relevant, comprehensive and up-to-date! Use the examples in the code as a starting basis for new routines; the output section corresponding to the various `autodoc` tags should be self-explanatory. See also Section 5.1.

The following files are used:

```
autodoc.f90
adheader.src
adfooter.src
```

To create the ($\sim$ 430) html files from the source code, type `make html`. Then, point your favourite web browser to the file `process.html` or `calling_tree.html` in the working directory. The variable descriptor file `vardes.html` (see Section 2.2) is also produced at the same time (though it may be helpful to modify the file manually afterwards to remove empty sections from it).

In addition, a full LaTeX User Guide (this document!), contained within `process.tex` and the other `.tex` files called from it, is rigorously maintained to ensure its continuing strict agreement with

the evolving source code. To create an Adobe PDF file `process.pdf` from `process.tex` (and the associated PostScript figures), type `make guide`.

Finally, to produce both the html files and the User Guide in one go, simply type `make doc`.

7.3 Code Updates and Release Procedure

This section describes the procedures that should be followed whenever new commits to the `develop` or `master` branches of the `PROCESS` Git repository are to be made, and how new code releases are performed. It is assumed that readers have a working knowledge of Git commands.

7.3.1 Initial access to the source code

To gain access to the `PROCESS` source code Git repository, you need to be given permission to do so via the CCFE `GitLab` server.

1. Use a web browser to go to `http://git.ccfe.ac.uk`
2. Login using your normal CCFE computer login details.
3. Assuming this is successful, contact the `GitLab PROCESS` "Owner" (currently James Morris james.morris2@cfe.ac.uk), who will add you to `GitLab` as a `PROCESS` "Developer".
4. (If this is your first access to `GitLab`, you may have to set up SSH keys and a few other things; follow the instructions on screen.)
5. Login to a Fusion Unix Network machine.
6. `cd SomewhereAppropriate` (you choose!)
7. `git clone git@git.ccfe.ac.uk:process/process.git -b develop my_develop` This copies the `develop` branch of the repository into a local folder `my_develop`, which will be created if it does not already exist.
8. `cd my_develop`
9. `git checkout develop`

   The sequence of commands above will provide you with a full copy of the `develop` branch of the `PROCESS` source code, Python utilities and all the documentation files.
10. `make all`
    This performs a full compilation and builds the executable, creates the User Guide, creates the python dictionaries and produces all the web-based documentation.

7.3.2 Git workflow

The code management methodology is based on the so-called "gitflow" workflow. There are two main branches:

- `develop`, which is the basis for all code development work, and changes are committed to it frequently.

- `master`, which contains official "release" versions of `PROCESS`, and is updated on a roughly three-monthly timescale.

Development work on new models should use separate branches, named e.g. `dev_mynewmodel`, split from the `develop` branch. It is a very good idea to merge the `develop` branch into `dev_mynewmodel` frequently during the course of the work, so that changes to the main branch are transferred to the new model's files with minimal effort.

Once the new model has been finished and tested successfully (complete with full documentation — see Section 5.1), the branch should be merged back into the `develop` branch.

7.3.2.1 Branching from `develop`

The following commands create a new branch in which to work on a new model. We assume that you are already in the `process` directory created above (Section 7.3.1).

1. `git checkout develop` (just to ensure that this is the branch *from which* you will be branching)
2. `git branch dev_mynewmodel`
3. `git checkout dev_mynewmodel`
4. `git push origin HEAD` (updates the central `GitLab` repository)

7.3.2.2 Working on a new model

Edit your local copies of the files as necessary. Whenever you want to save the changes back to the repository (it is prudent to do this at the end of each working day, as well as when the changes are complete, the code compiles and all test runs are successful!), use the following commands:

1. `git status` (this will show a list of modified files)
2. `git add changedfile1 changedfile2 ...`
   (This 'stages' the modified files marking them as ready for committing).
   `git commit`

   Alternatively, just use
   `git commit -a`
   This commits all modified tracked files.
3. An editor window will open; add a line summarising the changes you have made, save and close the window. This will initiate the commit to your *local* copy of the repository.
4. `git push`
   Copies the changes you have made locally to the version in the central `GitLab` repository. This uses a merging process, but if no-one else has changed your branch then the central version will simply become a copy of your local version.

7.3.2.3 Merging `develop` into working branch

It is a good idea to periodically merge the `develop` branch into the branch in which you are working, to ensure that any changes made in `develop` are included in your working branch.

1. Firstly, make sure you have committed your latest changes into the central `GitLab` repository as described in the previous section. Set the directory containing the working branch as your current directory.

2. `git pull`.
   Merges the version in the central repository into the local branch by copying over any changes that have been made in the version stored centrally.

3. `git checkout develop`
   This switches the "current branch" to `develop`.

4. `git pull`
   Updates the current branch of the local repository to the same branch on the central repository.

5. `git checkout dev_mynewmodel`
   This switches the "current branch" to `dev_mynewmodel`.

6. `git merge develop`
   Merges `develop` into the `dev_mynewmodel` branch.

7. Look for messages on the screen containing the word "conflict" indicating that some files cannot be merged directly. This typically happens if the same (or very closely-spaced) lines have been edited in both the `develop` and `dev_mynewmodel` branches.

   If any files are affected, they will be listed. Edit them and look for any lines containing `=======`. Such lines separate the changes made in the two branches, as in:

   ```
   <<<<<<< HEAD
   This line was edited in dev_mynewmodel branch
   =======
   This line was edited in develop branch
   >>>>>>> develop
   ```

   Resolve the conflict(s) as necessary. Then type `git add file1 file2 ...`, where `file1` etc. are the names of the files you removed conflicts from. Finally type `git commit` and edit the change log file.

8. `git push`
   Updates the central repository.

7.3.2.4 Merging working branch back into `develop`

Once the work on a model has been completed, fully tested and documented, the working branch should be merged back into the `develop` branch. This is done almost exactly as in the previous section, but there are a few crucial differences:

1. Firstly, make sure you have committed your latest changes to the working branch into the central `GitLab` repository.

2. `git pull`
   Merges the version in the central repository into the local branch by copying over any changes that have been made in the version stored centrally.

3. `git checkout dev_mynewmodel`

4. `git checkout develop`
5. `git merge dev_mynewmodel`
6. Look for any conflicts and resolve them as described in the previous section.
7. `git push`

7.3.2.5 Committing changes to `develop`

Whenever a commit to the `develop` branch is to be made, the following procedure should be followed. Ensure all documentation is up to date (see Section 5.1).

1. In routine `inform` of file `process.f90`, change the definition of `progver` by incrementing the revision number by one to `XYZ` (for instance) and the Release Date. It is important to keep exactly the same format.
2. Add a brief comment to the bottom of source file `process.f90` describing the changes made since the last commit in the same branch. Start the line with `!  GIT XYZ:` , following the existing examples.
3. If any of the User Guide `.tex` files have been modified, edit the definition of `\version` in `process.tex` by changing the Revision (to `XYZ`) and the date.
4. If you have changed any "use" statements in the code, or any compilation dependencies in the Makefile, run
   `make clean`
5. `make all`
   This ensures that all the code and documentation compiles successfully.
6. Run the input file(s) in the `tests` folder to ensure PROCESS runs correctly.
7. Close all open editor windows. The commit will not work otherwise.
8. `git commit -a`
   This commits all modified tracked files.

   Alternatively, you can this in two steps:
   `git add process.f90 process.tex changedfile1 changedfile2 ...`
   (This 'stages' the modified files marking them as ready for committing).
   `git commit`
9. An editor window will open; add a line summarising the changes you have made. Use a format like this:

   ```
   rXYZ    A summary of the changes made
   Further details. Changes due to Git issues can be described like this:
   #270    Description
   #273    Description
   ```

   Save and close the window. This will initiate the commit to your *local* copy of the repository.
10. `git tag -a rXYZ -m 'Revision XYZ'`

11. `git push`
12. `git push origin rXYZ`

The instructions given in Section 7.3.3 should now be followed to make the new `develop` release available to all users.

7.3.2.6 Merging develop into master

(to follow)

7.3.3 Full code rebuild

The standard `PROCESS` executables and the corresponding documentation available to all users are stored in the functional account called `PROCESS` on the CCFE Fusion Unix Network. Whenever the `master` or `develop` branches are updated a full rebuild of the standard executables and documentation should be performed. This is done as follows:

1. Ensure that all key users have been informed (using the commit message described above or directly).
2. `alter PROCESS` (this changes your current login to that of the `PROCESS` user; only registered individuals are able to do this)
3. `cd develop` (or `cd master`, as appropriate to the branch to be rebuilt)
4. `git pull`
   Updates the version stored in this folder to the version stored centrally.
5. `make all` This is essential because the Git repository does not include any of the files generated in the compilation process.
6. `exit` (to return to your own username again)

The `make all` step performs the rebuild of the `process.exe` executable file, updates the User Guide and all the html files, and recreates the Python dictionaries as required by the Python utilities.

Chapter 8

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Appendix A

The Optimisation Solver Explained

To give the user a better understanding of the optimisation solver implemented in `PROCESS` and the interpretation of its results, we give a short introduction into the mathematical background for solving these type of problems as well as the specific algorithm used.

In section A.1, the general nonlinear programming problem is defined, which is the mathematical description of our problem. This problem is typically formulated using Lagrange multipliers (c.f. A.2) and is solved numerically most efficiently using sequential quadratic programming (c.f. A.3). The Fortran subroutine that is used to implement such an optimisation solver in `PROCESS` is called `VMCON` (c.f. A.4), which iterates between solving a local quadratic subproblem (c.f. A.5) and a one dimensional line search (c.f. A.6). As the method uses a quasi-Newtonian approach the Hessian matrix is approximated by a variant of the Broyden-Fletcher-Goldfarb-Shanno update (A.7). Section A.8 summarises the symbol convention used in this chapter.

A.1 The General Nonlinear Programming Problem

Mathematically the *general nonlinear programming problem* or *nonlinear constrained optimisation problem* is defined as

$$\text{minimise } f(\boldsymbol{x}), \tag{A.1a}$$

$$\text{subject to } c_i(\boldsymbol{x}) = 0, \qquad i = 1, \ldots, k, \tag{A.1b}$$

$$\text{and } c_i(\boldsymbol{x}) \geq 0, \qquad i = k+1, \ldots, m, \tag{A.1c}$$

where both the *objective function*[1] $f(\boldsymbol{x})$ and the *constraints* $c_i(\boldsymbol{x})$ are nonlinear functions of the n-dimensional vector of variables $\boldsymbol{x}$ with bounds $\boldsymbol{x} \in \Omega$. In this context, all $\boldsymbol{x} \in \Omega$ that fulfill the constraints $c_i(\boldsymbol{x})$ are called *feasible*. They describe the allowed space in which we are trying to optimise the objective function $f(\boldsymbol{x})$. Note that any maximisation problem can be written as a minimisation by using $f_{\text{new}}(\boldsymbol{x}) = -f(\boldsymbol{x})$ and that any equality constraint $c(\boldsymbol{x}) = a$ can be rewritten as $c_{\text{new}}(\boldsymbol{x}) = c(\boldsymbol{x}) - a = 0$. Any inequality constraint can therefore be rearranged analogously to fit the form described in eq. A.1c.

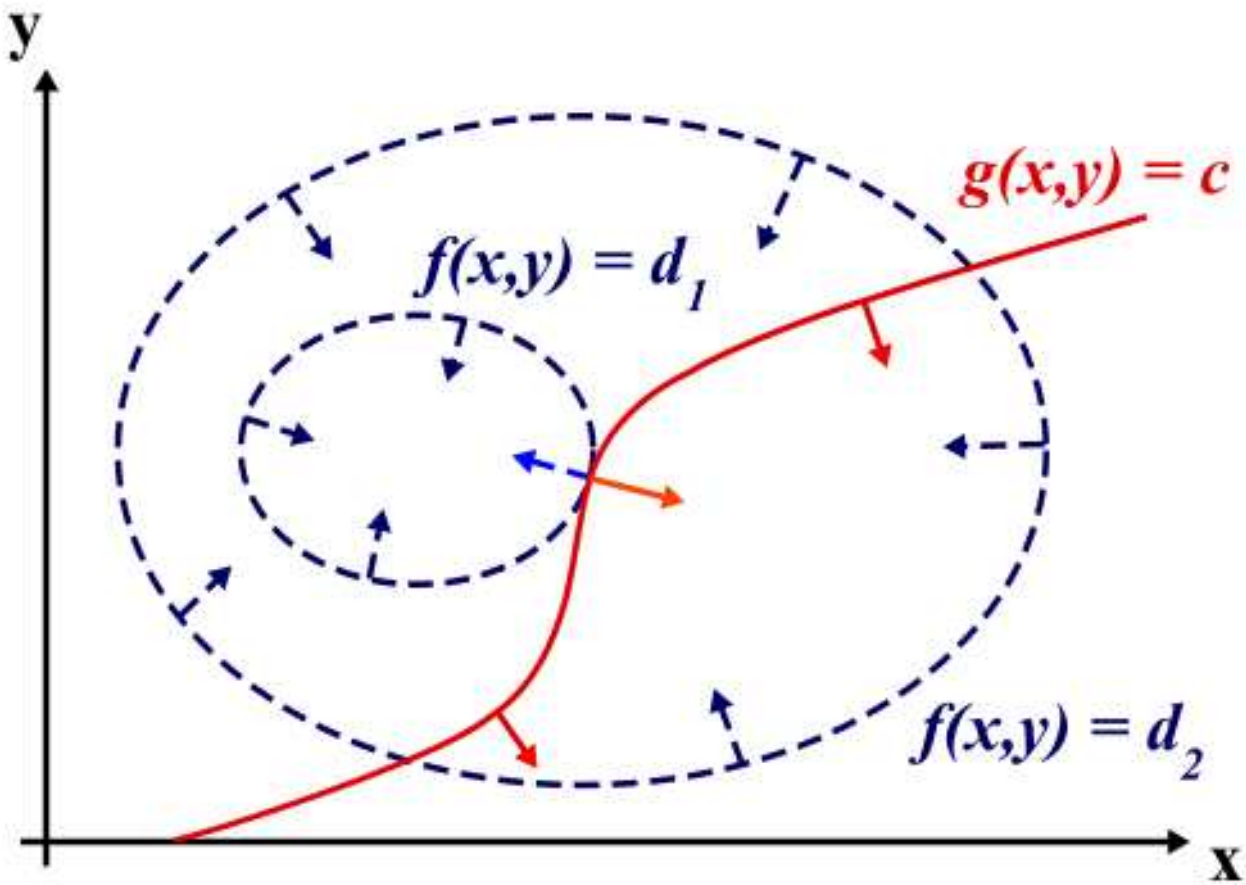

Figure A.1: *Illustration of Lagrange Multiplier Method (credit Wikipedia) showing two contour lines of the objective function $f(x, y) = d_i$ (dark blue dashed lines) and the nonlinear constraint $g(x, y) = c$ (red solid line) as well as their gradients (blue and red arrows) at various positions including the constrained optimum (light blue and orange arrows).*

A.2 The Lagrange Method

The general nonlinear programming problem can be solved mathematically using Lagrange's method. It assumes that the constraints cannot be used to explicitly reduce the parameter space of the iteration variables - as it is typically the case for non-linear constraints and objective functions - and is therefore a powerful method applicable to a general class of problems.

If we assume for simplicity that we have a 2D problem with only one equality constraint $c(x, y) = 0$, we know that we only need to search for the optimum along that constraint. At the optimum, the value of the objective function will then be stationary, i.e. it does not locally increase or decrease along the constraint. As the gradient of a function is perpedicular to its contour lines of $f(x, y) = d$, this is equivalent to saying that the gradient of the objective function at that point is parallel to the gradient of the constraints:

$$\nabla f(x, y) = -\lambda \nabla c(x, y), \tag{A.2}$$

where the factor λ is necessary as only the direction, but not the magnitude nor the sign of the gradients need to be equal. This is also illustrated in Figure A.1.

When expanding the method to several equality and inequality constraints we can make use of the *Lagrange function*. For the nonlinear programming problem described by A.1 it is given by

$$L(\boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{x}) - \sum_{i=1}^{m} \lambda_i c_i(\boldsymbol{x}), \tag{A.3}$$

with the corresponding *Lagrangian multipliers* λ_i. It allows us to formulate the *first order necessary* conditions for a constrained optimum $\boldsymbol{x}^*$ with corresponding Lagrange multipliers $\boldsymbol{\lambda}^*$, the Karush-Kuhn-Tucker (KKT) conditions,

$$\nabla_x L(\boldsymbol{x}^*, \boldsymbol{\lambda}^*) = \nabla_x f(\boldsymbol{x}^*) - \sum_{i=1}^{m} \lambda_i \nabla_x c_i(\boldsymbol{x}^*) = 0, \tag{A.4a}$$

$$\lambda_i^* c_i(\boldsymbol{x}^*) = 0, \qquad i = 1, \ldots, m, \tag{A.4b}$$

$$c_i(\boldsymbol{x}^*) = 0, \qquad i = 1, \ldots, k, \tag{A.4c}$$

$$\lambda_i^* \geq 0, \qquad i = k+1, \ldots, m, \tag{A.4d}$$

$$c_i(\boldsymbol{x}^*) \geq 0, \qquad i = k+1, \ldots, m. \tag{A.4e}$$

Please note that by construction the Lagrange multipliers λ_i^* fulfilling the KKT conditions are describing the derivative of the objective function with respect to the constraint equation $\frac{df}{dc_i}$ and are therefore a measure of how much the objective function changes with respect to each constraint.

In the special case of a *continuously differentiable convex* objective function $f(\boldsymbol{x})$ and equality constraints as well as *affine* inequality constraints, these KKT conditions are also sufficient for a global optimum. The `PROCESS` optimisation solver has been designed to converge on the KKT conditions, but does not test whether these are *sufficient* for a global optimum. It is therefore crucial that the user verifies that a global optimum has been found.

Furthermore, these conditions and therefore the solver, assume that both the objective function and constraints are at least *first order continuously partially differential*, i.e. that their first order partial derivatives are all continuous functions. This might not always be the case in `PROCESS` and is a potential source of errors.

[1] Please note that what is called *figure of merit* in `PROCESS` is called *objective function* in the mathematical optimisation context. Hence, both names are used equivalently in this document.

A.3 Sequential Quadratic Programming (SQP)

Based on the Lagrange method, sequential (also successive or recursive) quadratic programming is the most efficient method to numerically solve constrained nonlinear optimisation problems [74]. It combines a simple solver for a quadratic optimisation problem with linear constraints that determines a search direction $\boldsymbol{\delta}$ with a line search to find an optimum along that search direction. It is a type of the more general *feasible direction* methods which is itself a type of *primal method* that solve nonlinear programming problems in the $n - m$ dimensional feasible subspace [75].

A.4 VMCON

The optimisation solver implemented in PROCESS is the Fortran routine VMCON [5]. It is a modified version of the vf02ad routine from the Harwell Software Library[2] and implements a SQP method originally suggested by Powell[3] [6] based on work by Han [77]. As stated before VMCON is designed to converge on a solution of the *necessary* KKT conditions A.4, but does not check the *sufficient* conditions. Its convergence criterion is therefore given by

$$\left|\nabla_x f(\boldsymbol{x}^{j-1})^T \cdot \boldsymbol{\delta}^j\right| + \sum_{i=1}^{m} \left|\lambda_i^j c_i(\boldsymbol{x}^{j-1})\right| < \texttt{epsvmc} \tag{A.5}$$

where epsvmc is a user specified error tolerance, $\boldsymbol{\delta}^j$ is the vector in direction of the next line search (c.f. section A.6) and j is the counter of the sequential quadratic programming iteration. Hence, the first part estimates the predicted improvement due to the next line search and the second part measures the error in the complimentary condition A.4b of the KKT conditions.

Figure A.2 describes the flow chart of the VMCON routine, while the various values of the return parameter ifail[4] are described and interpreted in Table A.1.

A.5 The Quadratic Subproblem (QSP)

Within sequential quadratic programming the complex nonlinear problem is broken down into solving a sequence of local quadratic subproblems with linear constraints. This is based on the assumption that locally the problem is well approximated by a second order Taylor expansion of the Lagrange function. Hence, the local quadratic subproblem is described by

$$\text{minimise } Q(\boldsymbol{\delta}) = f(\boldsymbol{x}^{j-1}) + \boldsymbol{\delta}^T \nabla_x f(\boldsymbol{x}^{j-1}) + \frac{1}{2}\boldsymbol{\delta}^T \nabla_{xx} L(\boldsymbol{x}^{j-1}, \boldsymbol{\lambda}^{j-1})\boldsymbol{\delta} \tag{A.6a}$$

$$\text{subject to } \boldsymbol{\delta}^T \nabla_x c_i(\boldsymbol{x}^{j-1}) + c_i(\boldsymbol{x}^{j-1}) = 0,\ i = 1, \ldots, k, \tag{A.6b}$$

$$\text{and } \boldsymbol{\delta}^T \nabla_x c_i(\boldsymbol{x}^{j-1}) + c_i(\boldsymbol{x}^{j-1}) \geq 0,\ i = k+1, \ldots, m, \tag{A.6c}$$

where $\boldsymbol{\delta} = \boldsymbol{x} - \boldsymbol{x}^{j-1}$, the index $j - 1$ indicates the parameter values of the previous iteration[5] and $\nabla_{xx} L(\boldsymbol{x}^{j-1}, \boldsymbol{\lambda}^{j-1})$ is the Hessian of the Lagrange function. The solution of the QSP $\boldsymbol{\delta}$ describes the change of the current iteration variable vector that minimises the local approximation of the problem. To assure convergence even from bad starting points, it is not directly used to update the iteration

[2] www.hsl.rl.ac.uk

[3] This should not be confused with Powell's algorithm [76] which solves a multidimensional unconstrained minimisation problem without derivatives.

[4] Note, within the VMCON routine ifail is called info.

[5] Note j is called nqp in the VMCON routine.

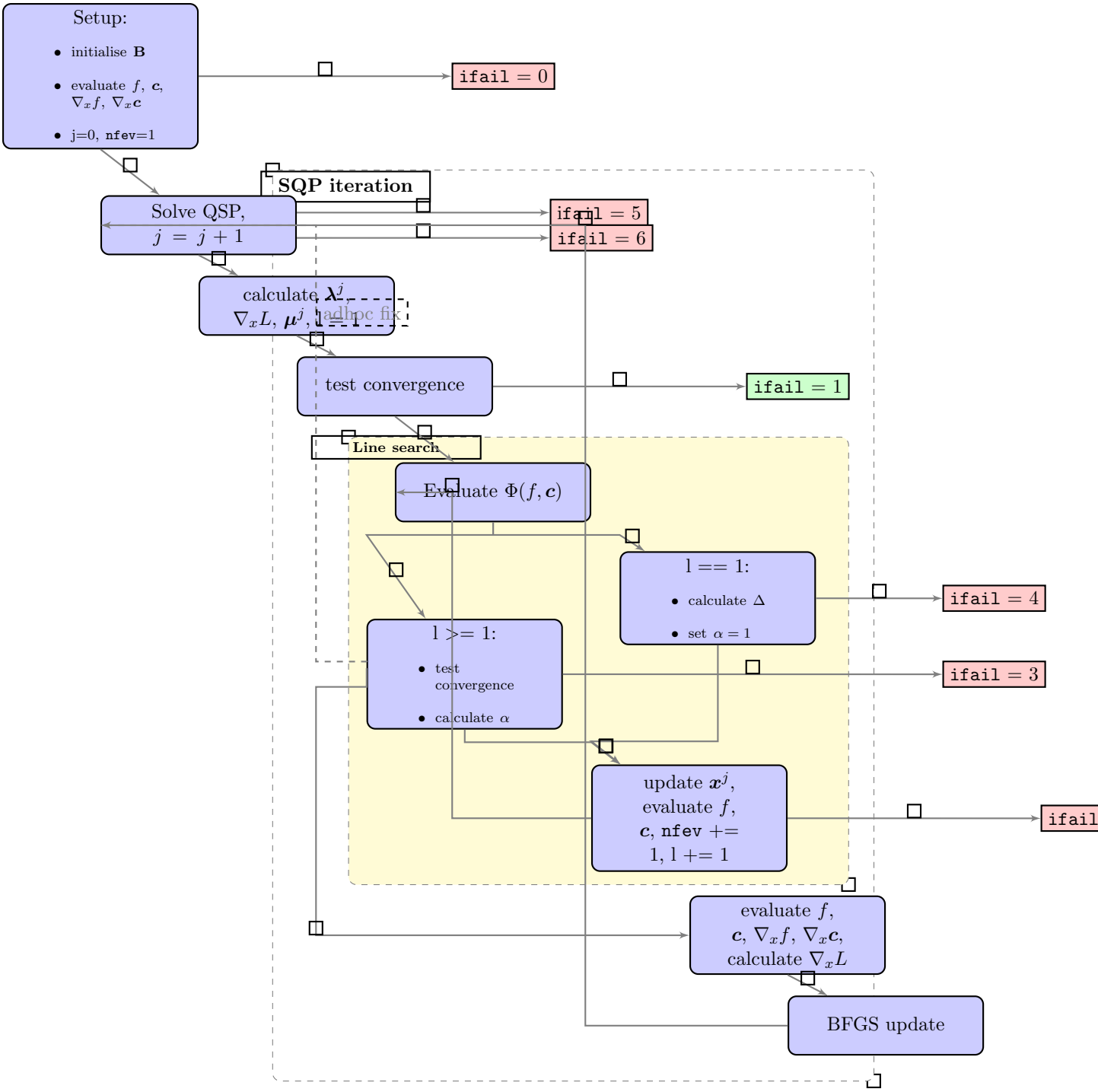

Figure A.2: *This is the flow chart of the* `VMCON` *optimisation solver. The criteria for and the interpretation of the successful (*`ifail` *= 1) and unsuccessful (*`ifail` *≠ 1) return parameters are described in Table A.1.*

`ifail`	Description	Meaning	Recommendation
0	`VMCON`: Improper input parameters	The input parameters to the solver are wrong, e.g. negative number of iteration variables.	This needs to be fixed on the developer side and should only occur in the test phase of new modules.
1	`VMCON`: Normal return	`VMCON` has found a solution that fulfills the necessary conditions within the specified error tolerances (c.f. eq. A.5).	Test whether the solution is a global solution by using different starting parameters.
2	Too many function calls	During the line search `VMCON` has reached the maximum number of total function calls (`maxfev`=100)	`VMCON` struggles to find a solution. Retry with different start parameters.
3	Line search required 10 functions calls	The results produced by input objective function/constraints and their gradients are inconsistent. This can be due to numerical noise in the input functions.	The developer needs to check the consistency and numerical robustness of the objective function, constraints and their derivatives. Perhaps the accurracy in numerical integrations/differentiations needs to be higher. As a user, try changing the iteration bounds or adding other iteration variables.
4	Uphill search direction was calculated	The quadratic subproblem has suggested a search direction in which the objective function only increases.	This happens if an inconsistency between the objective function, the constraints and their respective derivatives occurs (c.f. `ifail` =3).
5	`qpsub`: No feasible solution or bad approximation of Hessian	Either no optimum lies within the space allowed by the constraints and variable bounds or the identity matrix is not a good first approximation of the Hessian.	As a user, add a new iteration variable, as developer, try using a multiple of the identity matrix as initial Hessian instead.
6	`qpsub`: Singular matrix in quadratic subproblem or restriction by artificial bounds	This is fairly self-explanatory.	If this is meaningful, widen the boundaries of the iteration variables.

Table A.1: Summary of the description and meaning of the `VMCON` return parameters `ifail`.

variable vector, but describes the direction of the line search in which a 1d function is minimised using a Newtonian method (c.f. section A.6). Being a second order approximation to the original problem, it typically has a faster convergence that sequential linear programming (SLP) methods [78, chap. 10.4].

To allow the applicability of the solver to more general problems, Powell [6] substituted the Hessian $\nabla_{xx}L(\boldsymbol{x}^{j-1}, \boldsymbol{\lambda}^{j-1})$ with a positive definite approximation $\mathbf{B}$. This means that both the objective function $f(\boldsymbol{x})$ and the constraint equations $c_i(\boldsymbol{x})$ only have to be continuously differentiable instead of twice continuously differentiable with respect to the iteration variable vector $\boldsymbol{x}$. This makes the method a Quasi-Newtonian method as opposed to true Newtonian methods. How this approximation is initialised and updated is described in more detail in the section about the Broyden-Fletcher-Goldfarb-Shanno update A.7.

To solve the QSP `VMCON` uses `harwqp` a modification of the the Harwell library routine `VE02AD`, which in itself uses the subroutine `harwfp/LA02AD` to find a feasible point within the variable bounds and linearised constraints. Both routines go back to a method by Fletcher [79, 80, 81]. The Lagrange multipliers are also determined from results of the `harwqp` routine.

If the routine cannot find a feasible point it fails with `ifail` = 5 (c.f. Table A.1). As the routine is only checking the local linear approximation of the constraints rather the full non-linear constraints, there is a chance that a feasible point exists even though the routine fails with `ifail` = 5. In these cases, it is possible that the first approximation of the Hessian has not been good and the algorithm has, therefore, taken an inappropriately large step. Then using a multiple of the identity matrix will improve convergence of the algorithm.

If a singular matrix is encountered with the QSP solver or the solution is restricted by the artificial bounds, `VMCON` fails with `ifail` = 6. In this case it can be helpful to widen the boundaries of the iteration variables.

A.6 The Line Search

The line search is an essential part of the SQP algorithm. As Powell [6] pointed out, it is necessary to allow convergence from poor starting conditions. It uses the vector $\boldsymbol{\delta}$ from the QSP to update $\boldsymbol{x}^j = \boldsymbol{x}^{j-1} + \alpha^j \boldsymbol{\delta}^j$ where the step-length parameter $\alpha^j > 0$ is determined by the line search as the parameter that minimises

$$\Phi(\alpha) = f(\boldsymbol{x}) + \sum_{i=1}^{k} \mu_i \left|c_i(\boldsymbol{x})\right| + \sum_{i=k+1}^{m} \mu_i \left|min(0, c_i(\boldsymbol{x}))\right| \tag{A.7}$$

where the weights are defined as

$$\mu_i = \begin{cases} |\lambda_i^1| & \text{if } j = 1, \\ max\left(|\lambda_i^j|, 1/2(\mu_i^{j-1} + |\lambda_i^j|)\right) & \text{if } j > 1 \end{cases} \tag{A.8}$$

to assure maximally efficient convergence [77]. Note, that in this method locally *inactive* inequality constraints (c.f. 2.5.2) are not having any effect. It should always be possible, to find a solution that fulfills

$$\Phi(\alpha = 0) > \Phi(\alpha^j), \tag{A.9}$$

if

$$\left.\frac{d\Phi}{d\alpha}\right|_{\alpha=0} < 0. \tag{A.10}$$

In case the derivative is positive (`dflsa` ≥ 0), an uphill search direction has been determined and the code stops with `ifail` $= 4$. This typically only happens, if the objective function or constraints are inconsistent with their own derivatives.

As the line search tries to determine the optimum of a one dimensional, but fully non-linear function $\Phi(\alpha)$, it creates a series of α_l values[6]. At each iteration l, a quadratic local function $\Phi_l(\alpha)$ fullfilling the boundary conditions $\Phi_l(0) = \Phi(0)$, $\Phi_l'(0) = \Delta$ and $\Phi_l(\alpha_{l-1}) = \Phi(\alpha_{l-1})$ is minimised, where typically $\Delta = \Phi'(0)$. This leads to

$$\Phi_l(\alpha) = \Phi(0) + \Delta\alpha + \frac{\Phi(\alpha_{l-1}) - \Phi(0) - \Delta\alpha_{l-1}}{\alpha_{l-1}^2}\alpha^2 \tag{A.11}$$

and minimising this gives

$$\alpha_{min} = -\frac{\Delta\alpha_{l-1}^2}{2(\Phi(\alpha_{l-1}) - \Phi(0) - \Delta\alpha_{l-1})}. \tag{A.12}$$

Powell then sets $\alpha_l = \min(\alpha_{min}, 0.1\alpha_{l-1})$. On each iteration the convergence of the line search is tested. It is reached, if

$$\Phi(\alpha_l) - \Phi(0) < 0.1\Delta. \tag{A.13}$$

which assures that the change in the function is small in comparison to its derivative and 0.1 is a factor determined by experience. If this criterion is successful, the code exits the line search and updates all function evaluations.

As a modification to the original code, we have added an adhoc fix that exits the line search in the case of

$$\Phi(\alpha_l) - \Phi(0) > 0. \tag{A.14}$$

This has been added as experience have shown that `VMCON` typically does not converge in these situations, but if it is forced to caculate a new search direction in this way, it sometimes successfully finishes. Note, that this cannot force `VMCON` to converge on any false solutions, as it only exits positively when the convergence criterion A.5 is fulfilled.

Typically, the line search already converges after one iteration and, therefore, $\alpha = 1$. Hence, the `VMCON` line search has an upper limit of maximally 10 iterations before it terminating with `ifail` $= 3$ (c.f. Table A.1). This is higher than Powell's original limit of 5 to avoid a few cases of early termination without a major effect on efficiency.

Within the line search `VMCON` also checks that the total number of function calls has not exceeded `maxfev` $= 100$. If this is the case, it exits with error code `ifail` $= 2$. Both checks assure that the routine stops, if it does not seem to be able to find a solution.

A.7 The Broyden-Fletcher-Goldfarb-Shanno (BFGS) quasi-Newton update

`VMCON` uses a quasi-Newtonian update, the Broyden-Fletcher-Goldfarb-Shanno update, in the approximation of the Hessian of the Lagrange function. This means it is applicable to all continuously differentiable objective and constraint functions. Note, that due to the constraints it is not actually necessary for the Hessian of the solution to be positive definite, even though this is essential for the convergence of the algorithm.

In quasi-Newtonian methods the identity matrix $\mathbf{I}$ is often chosen as an initial estimate of the Hessian because of its positive definiteness. In some cases it can be helpful to chose a constant multiple of the

[6] In the actual code $\alpha =$`calpha` and $\alpha_l =$`alpha`$*\alpha_{l-1}$.

identity matrix instead. The BGFS update [7] is one way of revising the initial Hessian approximation using the update of the iteration variable vector

$$\boldsymbol{\xi} = \boldsymbol{x}^j - \boldsymbol{x}^{j-1} \tag{A.15}$$

and the update of the Jacobian of the Lagrange function

$$\boldsymbol{\gamma} = \nabla_x L(\boldsymbol{x}^j, \boldsymbol{\lambda}^j) - \nabla_x L(\boldsymbol{x}^{j-1}, \boldsymbol{\lambda}^j). \tag{A.16}$$

Note that unless $\alpha = 1$ in the line search, $\boldsymbol{\xi} \neq \boldsymbol{\delta}$. To assure the positive definiteness of $\mathbf{B}$ Powell [6] suggested a variation of the standard formalism that uses $\boldsymbol{\eta}$ instead of $\boldsymbol{\gamma}$

$$\boldsymbol{\eta} = \theta\boldsymbol{\gamma} + (1-\theta)\mathbf{B}\boldsymbol{\xi} \tag{A.17}$$

with

$$\theta = \begin{cases} 1 & \boldsymbol{\xi}^T\boldsymbol{\gamma} \geq 0.2\boldsymbol{\xi}^T\mathbf{B}\boldsymbol{\xi} \\ \frac{0.8\boldsymbol{\xi}^T B\boldsymbol{\xi}}{\boldsymbol{\xi}^T} & \boldsymbol{\xi}^T\boldsymbol{\gamma} < 0.2\boldsymbol{\xi}^T\mathbf{B}\boldsymbol{\xi} \end{cases} \tag{A.18}$$

to calculate a new approximation of the Hessian

$$\mathbf{B}_{new} = \mathbf{B} - \frac{\mathbf{B}\boldsymbol{\xi}\boldsymbol{\xi}^T\mathbf{B}}{\boldsymbol{\xi}^T\mathbf{B}\boldsymbol{\xi}} + \frac{\boldsymbol{\eta}^T\boldsymbol{\eta}}{\boldsymbol{\xi}^T\boldsymbol{\eta}}. \tag{A.19}$$

Using the modified version of the BFGS update as suggested by Powell, furthermore, assures superlinear convergence, even if the true Hessian is indefinite [82].

A.8 Symbols

In the previous sections the following conventions have been assumed: $\boldsymbol{x}$, $\boldsymbol{\delta}$, $\boldsymbol{\xi}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\eta}$ are n-dimensional vectors, where n is the number of iteration variables. $\boldsymbol{c}$, $\boldsymbol{\lambda}$, $\boldsymbol{\mu}$ are m-dimensional vectors, where m is the total number of constraints and c_i, λ_i and μ_i $(i = 1 \ldots m)$ are their respective components. $\mathbf{B}$ and $\mathbf{I}$ are $n \times n$-dimensional matrices, while $\nabla_x \boldsymbol{c}$ is an $n \times m$-dimensional matrix.

Appendix B

The Input File

The input file `IN.DAT` is used to change the values of the physics, engineering and other code parameters from their default values, and to set up the numerics (constraint equations, iteration variables etc.) required to define the problem to be solved. The user interface writes the input file, so it is not necessary to edit it directly.

B.0.1 Tokamak, stellarator, RFP or IFE?

The default model is the tokamak. To select a stellarator, reversed field pinch or inertial fusion energy plant, an additional input file is required, `device.dat`, which should contain a single character in the first line, which is interpreted as follows:

`0` : use tokamak model
`1` : use stellarator model
`2` : use reversed field pinch model
`3` : use inertial fusion energy model

B.0.2 File format

Variables can be specified in any order in the input file. Comment lines start with a `*` character. Data lines are of the form

```
variable = value
```

where `variable` is the name of one of the input parameters or iteration variables listed in the variable descriptor file, and `value` is the (usually numerical) initial value required for that variable. (Arrays, as opposed to scalar quantities, are treated differently — see below.) All input data are screened for non-sensible values.

The following rules must be obeyed when writing an input file:

1. Each variable must be on a separate line.
2. Variable names can be upper case, lower case, or a mixture of both.
3. Spaces may not appear within a variable name or data value.

4. Other spaces within a line, and trailing spaces, are ignored.
5. Commas are not necessary between variables (but see below).
6. Data can extend over more than one line.
7. One-dimensional arrays can be explicitly subscripted, or unscripted, in which case the following element order is assumed: `A(1), A(2), A(3),...`
8. At present, multiple dimension arrays can only be handled without reference to explicit subscripts, in which case the following element order is assumed: `B(1,1), B(2,1), B(3,1),...` The use of the input file to specify multiple dimension array elements is prone to error.
9. Unscripted array elements must be separated by commas.
10. Blank lines are allowed anywhere in the input file.
11. Lines starting with a `*` are assumed to be comments.
12. Comment lines starting with five or more asterisks (i.e. `*****`) are reproduced verbatim in the output file. This feature is not recommended, as these comments are likely to become out of date. The user interface does not support this feature.
13. In-line comments are *usually* ignored, but there can be problems if one contains a comma (`,`). If this is the case, there must also be a comma after the variable's value and before the comment.

It is useful to divide the input file into sections, using suitable comment lines, to help the user keep related variables together.

The following is a valid fragment of an input file (the vertical lines are simply to help show the column alignment):

```
* This line is a comment that will not appear in the output
***** This line is a comment that will appear in the output
boundl(1) = 2.5,
BOUNDU(10) = 3.,
BOUNDU(45) = 1,
* Another comment...  Note that real values can be entered as if
* they were integers, and vice versa (but it's not recommended...)
epsfcn = 10.e-4,
Ftol = 1.D-4,
* The next line sets the first five elements of array icc:
ICC = 2, 10, 11, 24, 31
* The next line sets the first ten elements of array ixc:
ixc = 10, 12, 3, 36, 48,
       1, 2, 6, 13, 16,
IOPTIMZ = 1,
maxcal = 200
 nsweep = 7
NEQNS = 5, This is an in-line comment
NVAR = 10, Another, but successfully containing a comma!
```

The following are *invalid* entries in the input file (Q: Why?!):

```
boundl(1,1) = 2.5,
BOUNDU(N) = 3.,
A line of ‘random’ characters like this will clearly wreak havoc
eps fcn = 10.e-4, ftol = 1.D-4
epsvmc = 1.0 e-4
ICC = 2 10 11 24 31
IOPTIMZ = 1.0, This will in fact be okay - but is not recommended
NEQNS = 5 An in-line comment on a line with only one comma (,) character
```

If the code encounters a problem reading the input file, it will stop immediately with a (hopefully) useful error message. It may be worth looking at the contents of the output file as well, to help narrow down on which line of the input file the problem might lie.

Appendix C

Optimisation Input File

The following is a typical input file used to run PROCESS in optimisation mode.

```
*****
runtitle = 'Example input file'
*--------------------------------------------------*

*---------------Constraint Equations---------------*
neqns = 18
icc(1) = 1        * beta (consistency equation)
icc(2) = 2        * global power balance (consistency equation)
icc(3) = 5        * density upper limit
icc(4) = 8        * neutron wall load upper limit
icc(5) = 10       * toroidal field 1/r (consistency equation)
icc(6) = 11       * radial build (consistency equation)
icc(7) = 13       * burn time lower limit (pulse)
icc(8) = 15       * l-h power threshold limit
icc(9) = 16       * net electric power lower limit
icc(10) = 24      * beta upper limit
icc(11) = 26      * central solenoid eof current density upper limit
icc(12) = 27      * central solenoid bop current density upper limit
icc(13) = 30      * injection power upper limit
icc(14) = 31      * tf coil case stress upper limit (sctf)
icc(15) = 32      * tf coil conduit stress upper limit (sctf)
icc(16) = 33      * i_op / i_critical (tf coil) (sctf)
icc(17) = 34      * dump voltage upper limit (sctf)
icc(18) = 35      * j_winding pack/j_protection upper limit (sctf)

*---------------Iteration Variables----------------*
nvar = 31
ixc(1) = 2        * bt * Toroidal field on axis (t) (iteration variable 2)
boundl(2) = 0.01
boundu(2) = 100.0

ixc(2) = 3        * rmajor * Plasma major radius (m) (iteration variable 3)
boundl(3) = 0.1
boundu(3) = 13.0

ixc(3) = 4        * te * Volume averaged electron temperature (kev)
boundl(4) = 5.0
boundu(4) = 150.0

ixc(4) = 5        * beta * Total plasma beta (iteration variable 5)
boundl(5) = 0.001
boundu(5) = 1.0
```

```
ixc(5) = 6        * dene * Electron density (/m3) (iteration variable 6)
boundl(6) = 1e+19
boundu(6) = 1e+21

ixc(6) = 9        * fdene * F-value for density limit
boundl(9) = 0.001
boundu(9) = 1.2

ixc(7) = 10       * hfact * H factor on energy confinement times (iteration variable 10)
boundl(10) = 0.1
boundu(10) = 1.1

ixc(8) = 12       * oacdcp * Overall current density in tf coil inboard legs (a/m2)
boundl(12) = 100000.0
boundu(12) = 150000000.0

ixc(9) = 13       * tfcth * Inboard tf coil thickness; (centrepost for st) (m)
boundl(13) = 0.5
boundu(13) = 5.0

ixc(10) = 14      * fwalld * F-value for minimum wall load
boundl(14) = 0.001
boundu(14) = 1.0

ixc(11) = 16      * ohcth * Central solenoid thickness (m)
boundl(16) = 0.001
boundu(16) = 100.0

ixc(12) = 18      * q * Safety factor 'near' plasma edge (iteration variable 18)
boundl(18) = 3.0
boundu(18) = 100.0

ixc(13) = 29      * bore * Central solenoid inboard radius (m)
boundl(29) = 0.1
boundu(29) = 10.0

ixc(14) = 36      * fbetatry * F-value for beta limit
boundl(36) = 0.001
boundu(36) = 1.0

ixc(15) = 37      * coheof * Central solenoid overall current density at end of flat-top (a/m2)
boundl(37) = 100000.0
boundu(37) = 100000000.0

ixc(16) = 38      * fjohc * F-value for central solenoid current at end-of-flattop
boundl(38) = 0.01
boundu(38) = 0.25

ixc(17) = 39      * fjohc0 * F-value for central solenoid current at beginning of pulse
boundl(39) = 0.001
boundu(39) = 0.25

ixc(18) = 41      * fcohbop * Ratio of central solenoid overall current density at
boundl(41) = 0.001
boundu(41) = 1.0

ixc(19) = 42      * gapoh * Gap between central solenoid and tf coil
boundl(42) = 0.05
boundu(42) = 0.1

ixc(20) = 44      * fvsbrnni * Fraction of the plasma current produced by
```

```
boundl(44) = 0.001
boundu(44) = 1.0

ixc(21) = 48      * fstrcase * F-value for tf coil case stress
boundl(48) = 0.001
boundu(48) = 1.0

ixc(22) = 49      * fstrcond * F-value for tf coil conduit stress
boundl(49) = 0.001
boundu(49) = 1.0

ixc(23) = 50      * fiooic * F-value for tf coil operating current / critical
boundl(50) = 0.001
boundu(50) = 0.5

ixc(24) = 51      * fvdump * F-value for dump voltage
boundl(51) = 0.001
boundu(51) = 1.0

ixc(25) = 53      * fjprot * F-value for tf coil winding pack current density
boundl(53) = 0.001
boundu(53) = 1.0

ixc(26) = 56      * tdmptf * Dump time for tf coil (s)
boundl(56) = 10.0
boundu(56) = 1000000.0

ixc(27) = 57      * thkcas * Inboard tf coil case outer (non-plasma side) thickness (m)
boundl(57) = 0.05
boundu(57) = 1.0

ixc(28) = 58      * thwcndut * Tf coil conduit case thickness (m)
boundl(58) = 0.004
boundu(58) = 1.0

ixc(29) = 59      * fcutfsu * Copper fraction of cable conductor (tf coils)
boundl(59) = 0.001
boundu(59) = 1.0

ixc(30) = 61      * gapds * Gap between inboard vacuum vessel and tf coil (m)
boundl(61) = 0.12
boundu(61) = 10.0

ixc(31) = 103     * flhthresh * F-value for l-h power threshold
boundl(103) = 1.0
boundu(103) = 1000000.0

*-----------------Build Variables------------------*
blnkith = 0.755  * Inboard blanket thickness (m);
blnkoth = 1.275  * Outboard blanket thickness (m);
bore = 2.5907    * Central solenoid inboard radius (m)
ddwex = 0.15     * External cryostat thickness (m)
ddwi = 0.32      * Vacuum vessel thickness (tf coil / shield) (m)
fwith = 0.025    * Inboard first wall thickness; initial estimate (m)
fwoth = 0.025    * Outboard first wall thickness; initial estimate (m)
gapds = 0.12     * Gap between inboard vacuum vessel and tf coil (m)
gapoh = 0.05     * Gap between central solenoid and tf coil
gapomin = 0.2    * Minimum gap between outboard vacuum vessel and tf coil (m)
ohcth = 0.86365  * Central solenoid thickness (m)
scrapli = 0.225  * Gap between plasma and first wall; inboard side (m)
scraplo = 0.225  * Gap between plasma and first wall; outboard side (m)
shldith = 0.3    * Inboard shield thickness (m)
```

```
shldoth = 0.8    * Outboard shield thickness (m)
shldtth = 0.3    * Upper/lower shield thickness (m);
tfcth = 0.79433  * Inboard tf coil thickness; (centrepost for st) (m)
vgap2 = 0.12     * Vertical gap between vacuum vessel and tf coil (m)
vgaptf = 1.6     * Vertical gap between x-point and divertor (m)


*---------------Buildings Variables----------------*


*---------------Constraint Variables---------------*
bmxlim = 14.0    * Maximum peak toroidal field (t)
fbetatry = 0.52645  * F-value for beta limit
fdene = 1.2      * F-value for density limit
fhldiv = 2.0     * F-value for divertor heat load
fjohc = 0.25     * F-value for central solenoid current at end-of-flattop
fjohc0 = 0.25    * F-value for central solenoid current at beginning of pulse
flhthresh = 1.0232  * F-value for l-h power threshold
fpeakb = 0.9229  * F-value for maximum toroidal field
fstrcond = 0.84986  * F-value for tf coil conduit stress
fvdump = 0.96778  * F-value for dump voltage
fwalld = 0.13514  * F-value for minimum wall load
pnetelin = 500.0  * Required net electric power (mw)
pseprmax = 17.0  * Maximum ratio of power crossing the separatrix to
tbrnmn = 7200.0  * Minimum burn time (s)
walalw = 8.0     * Allowable wall-load (mw/m2)


*------------------Cost Variables------------------*
abktflnc = 15.0  * Allowable first wall/blanket neutron
adivflnc = 20.0  * Allowable divertor heat fluence (mw-yr/m2)
fcap0 = 1.15     * Average cost of money for construction of plant
fcap0cp = 1.06   * Average cost of money for replaceable components
fcontng = 0.15   * Project contingency factor
fcr0 = 0.065     * Fixed charge rate during construction
ifueltyp = 1     * Switch * treat blanket divertor; first wall and
lsa = 2          * Level of safety assurance switch
output_costs = 0  * Switch for costs output * do not write cost-related outputs to file;
ratecdol = 0.06  * Effective cost of money in constant dollars
tlife = 40.0     * Plant life (years)
ucblvd = 280.0   * Unit cost for blanket vanadium ($/kg)
ucdiv = 500000.0  * Cost of divertor blade ($)
ucme = 300000000.0  * Unit cost of maintenance equipment ($/w**0;3)


*-------------Current Drive Variables--------------*
bscfmax = 0.99   * Maximum fraction of plasma current from bootstrap;
etanbi = 0.4     * Neutral beam wall plug to injector efficiency
frbeam = 1.0     * R_tangential / r_major for neutral beam injection
pinjalw = 50.0   * Maximum allowable value for injected power (mw)


*----------------Divertor Variables----------------*
anginc = 0.175   * Angle of incidence of field line on plate (rad)
divdum = 1       * Switch for divertor zeff model* 0=calc; 1=input
divfix = 0.621   * Divertor structure vertical thickness (m)
hldivlim = 10.0  * Heat load limit (mw/m2)
ksic = 1.4       * Power fraction for outboard double-null scrape-off plasma
prn1 = 0.4       * N-scrape-off / n-average plasma;
zeffdiv = 3.5    * Zeff in the divertor region (if divdum /= 0)
```

```
*------------------Fwbs Variables------------------*
fwclfr = 0.1     * First wall coolant fraction


*-----------------Global Variables-----------------*


*-------------Heat Transport Variables-------------*
etath = 0.375    * Thermal to electric conversion efficiency
fauxbop = 0.032  * Fraction of gross electric power to balance-of-plant
ffwlg = 0.01     * Fraction of first wall / divertor power to low grade heat
htpmw = 155.0    * Heat transport system electrical pump power (mw)


*------------------Ife Variables-------------------*


*------------Impurity Radiation Module-------------*
coreradius = 0.6  * Normalised radius defining the 'core' region
fimp = 1.0, 0.1, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.00044, 5e-05  * Impurity number density fracti
impvar = 13      * Fimp element value to be varied if iteration


*---------------------Numerics---------------------*
ioptimz = 1      * Code operation switch * for no optimisation; hybrd only;
minmax = 1       * Switch for figure-of-merit * major radius
epsvmc = 1e-08   * Error tolerance for vmcon


*----------------Pf Power Variables----------------*


*-----------------Pfcoil Variables-----------------*
coheof = 12994000.0  * Central solenoid overall current density at end of flat-top (a/m2)
cptdin = 42200.0, 42200.0, 42200.0, 42200.0, 43000.0, 43000.0, 43000.0, 43000.0  * Peak current per turn input for
fcohbop = 0.93314  * Ratio of central solenoid overall current density at
ipfloc = 2, 2, 3, 3  * Switch for locating scheme of pf coil group i
isumatpf = 3     * Switch for superconductor material in pf coils * nbti;
ncls = 1, 1, 2, 2  * Number of pf coils in group j
ngrp = 4         * Number of groups of pf coils;
ohhghf = 0.9     * Central solenoid height / tf coil internal height
rjconpf = 11000000.0, 11000000.0, 6000000.0, 6000000.0, 8000000.0, 8000000.0, 8000000.0, 8000000.0  * Average windi
rpf2 = -1.825    * Offset (m) of radial position of ipfloc=2 pf coils
sigpfalw = 300.0  * Allowable stress in pf coils/central solenoid (mpa)
zref = 3.6, 1.2, 1.0, 2.8, 1.0, 1.0, 1.0, 1.0  * Pf coil vertical positioning adjuster


*----------------Physics Variables-----------------*
alphaj = 2.0     * Current profile index;
alphan = 1.0     * Density profile index
alphat = 1.0     * Temperature profile index
aspect = 3.5     * Aspect ratio (iteration variable 1)
beta = 0.034253  * Total plasma beta (iteration variable 5)
bt = 5.3983      * Toroidal field on axis (t) (iteration variable 2)
dene = 8.2808e+19  * Electron density (/m3) (iteration variable 6)
dnbeta = 3.0     * (troyon-like) coefficient for beta scaling;
fkzohm = 1.0245  * Zohm elongation scaling adjustment factor (ishape=2; 3)
fvsbrnni = 0.43898  * Fraction of the plasma current produced by
gamma = 0.3      * Ejima coefficient for resistive startup v-s formula
hfact = 1.1      * H factor on energy confinement times (iteration variable 10)
ibss = 4         * Switch for bootstrap current scaling * for sauter et al scaling
iculbl = 1       * Switch for beta limit scaling * apply limit to thermal beta;
```

```
impc = 0.0       * Carbon impurity multiplier (imprad_model=0 only)
impo = 0.0       * Oxygen impurity multiplier (imprad_model=0 only)
neped = 6.78e+19  * Electron density of pedestal (/m3) (ipedestal=1)
nesep = 2e+19    * Electron density at separatrix (/m3) (ipedestal=1)
rhopedn = 0.94   * R/a of density pedestal (ipedestal=1)
rhopedt = 0.94   * R/a of temperature pedestal (ipedestal=1)
teped = 5.5      * Electron temperature of pedestal (kev) (ipedestal=1)
tesep = 0.1      * Electron temperature at separatrix (kev) (ipedestal=1)
ishape = 2       * Switch for plasma cross-sectional shape calculation * set kappa to the natural elongation value
kappa = 1.7      * Plasma separatrix elongation (calculated if ishape > 0)
rmajor = 8.9216  * Plasma major radius (m) (iteration variable 3)
te = 12.959      * Volume averaged electron temperature (kev)
triang = 0.5     * Plasma separatrix triangularity (calculated if ishape=1; 3 or 4)
zfear = 1        * High-z impurity switch; 0=iron; 1=argon


*-----------------Pulse Variables------------------*
lpulse = 1       * Switch for reactor model * pulsed operation


*------------------Rfp Variables-------------------*


*-------------------Scan Module--------------------*
isweep = 1       * Number of scan points to calculate
nsweep = 1       * Switch denoting quantity to scan * aspect
sweep = 3.1      * Actual values to use in scan


*--------------Stellarator Variables---------------*


*-----------------Tfcoil Variables-----------------*
casths = 0.05    * Inboard tf coil sidewall case thickness (m)
cpttf = 65000.0  * Tf coil current per turn (a)
csytf = 990000000.0  * Yield strength of case (tf coils and cs coils) (pa)
fcutfsu = 0.61471  * Copper fraction of cable conductor (tf coils)
oacdcp = 12367000.0  * Overall current density in tf coil inboard legs (a/m2)
ripmax = 0.6     * Maximum allowable toroidal field ripple amplitude
tfno = 18.0      * Number of tf coils (default = 50 for stellarators)
tftmp = 4.75     * Peak helium coolant temperature in tf coils and pf coils (k)
thicndut = 0.001  * Conduit insulation thickness (m)
thkcas = 0.43968  * Inboard tf coil case outer (non-plasma side) thickness (m)
thwcndut = 0.004  * Tf coil conduit case thickness (m)
tmargmin = 1.7   * Minimum allowable temperature margin (cs and tf coils) (k)
vftf = 0.333     * Coolant fraction of tf coil leg (itfsup=0)


*-----------------Times Variables------------------*
tburn = 10000.0  * Burn time (s) (calculated if lpulse=1)


*-----------------Vacuum Variables-----------------*
```

Appendix D

Non-optimisation Input File

The following is a typical input file used to run PROCESS in non-optimisation mode. Comments in [...] have been added to the right of each line.

```
* Numerics information                [Comment]

NEQNS = 14,                           [Number of active constraint equations]
NVAR = 14,                            [Number of active iteration variables]
ICC =   1,  2, 10, 11, 7, 16, 24, 5, 31, 32, 33, 34, 35, 36,  [Constraint eqns]
ixc =   5, 10, 12, 3,  7,  6, 36, 9, 48, 49, 50, 51, 53, 54,  [Iteration variables]
IOPTIMZ = -1,                         [Turn off optimisation]
ISWEEP=0                              [No scans (non-optimisation mode)]

* F-values and limits

FBETATRY = 1.0                        [N.B. active iteration variable 36]

* Physics parameters

ASPECT = 3.5,                         [Machine aspect ratio]
BETA = 0.042,                         [N.B. active iteration variable 5]
BT = 6.,                              [Toroidal field on axis]
DENE = 1.5e20,                        [N.B. active iteration variable 6]
FVSBRNNI = 1.0,                       [Non-inductive volt seconds fraction]
DNBETA = 3.5,                         [Beta g coefficient]
HFACT = 2.,                           [N.B. active iteration variable 10]
ICURR = 4,                            [Use ITER current scaling]
ISC = 6,                              [Use ITER 89-P confinement time scaling law]
IINVQD = 1,                           [Use inverse quadrature]
IITER = 1,                            [Use ITER fusion power calculations]
ISHAPE = 0,                           [Use input values for KAPPA and TRIANG]
KAPPA = 2.218,                        [Plasma elongation]
Q = 3.0,                              [Edge safety factor]
RMAJOR = 7.0,                         [N.B. active iteration variable 3]
RNBEAM = 0.0002,                      [N.B. active iteration variable 7]
TBURN = 227.9                         [Burn time]
TE = 15.,                             [Electron temperature]
TRIANG = 0.6                          [Plasma triangularity]

* Current drive parameters

IRFCD = 1,                            [Use current drive]
IEFRF = 5                             [Use ITER neutral beam current drive]
FEFFCD = 3.,                          [Artificially enhance efficiency]
```

```
* Divertor parameters

ANGINC=0.262,                          [Angle of incidence of field lines on plate]
PRN1=0.285                             [Density ratio]

* Machine build

BORE = 0.12,                           [Machine bore]
OHCTH = 0.1,                           [central solenoid thickness]
GAPOH = 0.08,                          [Inboard gap]
TFCTH = 0.9,                           [Inboard TF coil leg thickness]
DDWI = 0.07,                           [Vacuum vessel thickness]
SHLDITH = 0.69,                        [Inboard shield thickness]
BLNKITH = 0.115,                       [Inboard blanket thickness]
FWITH = 0.035,                         [Inboard first wall thickness]
SCRAPLI = 0.14,                        [Inboard scrape-off layer thickness]
SCRAPLO = 0.15,                        [Outboard scrape-off layer thickness]
FWOTH = 0.035,                         [Outboard first wall thickness]
BLNKOTH = 0.235,                       [Outboard blanket thickness]
SHLDOTH = 1.05,                        [Outboard shield thickness]
GAPOMIN = 0.21,                        [Outboard gap]
VGAPTF = 0,                            [Vertical gap]

* First wall, blanket, shield parameters

LBLNKT=0                               [Use old blanket model]
DENSTL=7800.                           [Steel density]

* TF coil parameters

OACDCP = 1.4e7,                        [N.B. active iteration variable 12]
ITFSUP = 1,                            [Use superconducting TF coils]
RIPMAX = 5.,                           [Maximum TF ripple]

* PF coil parameters

NGRP = 3,                              [Three groups of PF coils]
IPFLOC = 1,2,3,                        [Locations for each group]
NCLS = 2,2,2,1,                        [Number of coils in each group]
COHEOF = 1.85e7,                       [central solenoid current at End Of Flat-top]
FCOHBOP = 0.9,                         [central solenoid current at Begin. Of Pulse / COHEOF]
ROUTR = 1.5,                           [Radial position for group 3]
ZREF(3) = 2.5,                         [Z position for group 3]
OHHGHF = .71                           [Height ratio central solenoid / TF coil]

* Vacuum system parameters

NTYPE = 1                              [Use cryopump]

* Heat transport parameters

ETATH=0.35                             [Thermal to electric conversion efficiency]
FMGDMW = 0.                            [Power to MGF units]
BASEEL=5.e6                            [Base plant electric load]
ISCENR=2                               [Energy store option]

* Buildings

FNDT = 2.                              [Foundation thickness]
EFLOOR=1.d5                            [Effective total floor space]
```

```
* Costs

IREACTOR = 1,                          [Calculate cost of electricity]
IFUELTYP = 0                           [Treat blanket, first wall etc as capital cost]
UCHRS = 87.9,                          [Unit cost of heat rejection system]
UCCPCL1 = 250,                         [Unit cost of high strength tapered copper]
UCCPCLB = 150                          [Unit cost of TF outer leg plate coils]
```