A design and development procedure for transceive radio frequency coils in ultra-high field magnetic resonance

Doctoral thesis at the Medical University of Vienna for obtaining the academic degree

Doctor of Philosophy

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Symbols and Abbreviations

\(\gamma\) .............. Gyromagnetic ratio [MHz/T]
\(h\) .............. Reduced Planck constant = \(h/2\pi = 1.054571726(47) \cdot 10^{-34}\) [Js]
\(\kappa_B\) .............. Boltzmann constant = 1.3806488(13) \cdot 10^{-23} [J/K]
\(c\) .............. Speed of light = 299793458 [m/s]
\(\lambda\) .............. Wavelength [m]
\(B\) .............. Magnetic flux density [T]
\(B_0\) .............. Main/static magnetic flux density [T]
\(B_1\) .............. RF flux density [T]
\(B_1^+\) .............. Positively rotating RF field (transmit field) [T]
\(B_1^-\) .............. Negatively rotating RF field (receive field) [T]
\(E\) .............. Electric field [V/m]
\(H\) .............. Magnetic field [A/m]
\(\mathcal{C}\) .............. Computational domain
\(\mu_0\) .............. Permeability of free space = \(4\pi \cdot 10^{-7}\) [H/m]
\(\mu_r\) .............. Relative permeability
\(\varepsilon_0\) .............. Permittivity of free space = 8.854187817\ldots \cdot 10^{-12} [F/m]
\(\varepsilon_r\) .............. Relative permittivity
\(\rho_c\) .............. Total charge density [C/m]
\(\rho_m\) .............. Mass density [kg/m^3]
\(\sigma\) .............. Electrical conductivity [S/m]
$^1$H ............ Hydrogen-1 isotope
$^{31}$P ............ Phosphor-31 isotope
I ............... Spin quantum number
$m_I$ ............ Magnetic quantum number
SAR ............. Specific absorption rate [W/kg]
SNR ............. Signal-to-noise ratio
FDTD ............ Finite difference time domain method
NMR ............. Nuclear magnetic resonance
MRI ............. Magnetic resonance imaging
MRS ............. Magnetic resonance spectroscopy
Abstract

Nuclear magnetic resonance (NMR) forms the basis of magnetic resonance imaging (MRI) and spectroscopy (MRS), both of which are frequently used non invasive methods to gain insight into human physiology and anatomy. NMR utilizes the magnetic properties of atomic nuclei of biological tissues and their interactions with a main static magnetic field ($B_0$) and a time varying radio frequency (RF) field ($B_1$). For signal generation the RF field is irradiated by an RF coil, usually orthogonal to the main field direction. Spatial localization of the signal is then achieved via orthogonal field gradients. Magnetic resonance can be categorized as a low sensitivity method compared to other imaging methodologies like computer tomography (CT), or photon emission tomography (PET), due to the small number of signal producing nuclear spins. The available spatial and/or temporal resolution is often limited by the signal-to-noise ratio (SNR), which is proportional to the main magnetic field strength. As a rule of thumb: higher $B_0$ facilitates higher SNR, at the cost of more complex field interactions. This causes a continued trend towards higher field strengths to enable finer spatial resolution or faster acquisition.

The resonance frequency is dependent on the type of nucleus investigated, e.g. $^1$H, $^{23}$Na, $^{31}$P, and increases linearly with the main field strength, resulting in shorter wave lengths and therefore more complex electromagnetic (EM) fields produced inside the human body by the RF coils in use. This complexity creates the need for specifically optimized designs for RF probes operating in the ultra high field regime ($>3$ T). For optimization purposes, knowledge of the EM field distribution and amplitude is needed. Since the MR signal is sensitive to the RF coil's magnetic $B_1$ field, it can be visualized and quantified in the MR scanner. Unfortunately this is not true for the concomitant electric field ($E$). Although the $E$ field is not needed for MR, it has to be carefully evaluated, since it deposits energy inside conducting samples which results in tissue heating, and therefore, being a major safety issue. Numerical simulation of Maxwell’s equations enables the analysis of the produced EM fields before physically building a coil. In the last decades, EM simulations has proven to be an indispensable tool for RF coil design.

This work describes a feasible workflow for the development of RF coils for transmission and reception of MR signals. Special attention was paid to a comprehensive evaluation using numerical simulation, not only to optimize the design but also to ensure safety for future patient use. To assess the accuracy of the simulation results, various in-scanner validation methods are presented.

A $^{31}$P/$^1$H RF coil conformed to the human calf for $^{31}$P metabolic investigations of skeletal muscle in the human lower extremities before, during, and after exercise, was designed, developed and tested according to the presented workflow. Studies conducted with the developed RF coil are presented shortly, to underline the functionality of the built system.
Additional preliminary results of a second $^{31}\text{P}/^1\text{H}$ RF coil for $^{31}\text{P}$ metabolic investigations in the human occipital lobe are presented.
Zusammenfassung

Die Kernspinresonanz (NMR) bildet die Grundlage zur Magnetresonanztomographie (MRT), sowie der Kernspinresonanzspektroskopie (MRS). Sie ist ein häufig genutztes medizinisches Verfahren, um funktionelle und quantitative Informationen über die menschliche Physiologie und Anatomie in nicht-invasiver Weise zu erhalten. NMR nutzt dabei die magnetischen Eigenschaften von Atomkernen, enthalten in biologischen Geweben, und deren Wechselwirkung mit einem statischen Magnetfeld ($B_0$). Im Vergleich zu anderen bildgebenden Verfahren, wie Computertomographie (CT), oder Positronen-Emissions-Tomographie (PET), ist NMR als eher niedrig sensitiv einzuordnen, was an der geringen Anzahl an signalgebenden Kernspins liegt. Für die Signalanzeige wird ein zusätzliches Radiofrequenz (RF) Feld ($B_1$), produziert von einer RF Spule, eingestrahlt. Die Lokalisierung des Signals wird dann durch drei orthogonale Gradientenfelder ermöglicht. Die verfügbare örtliche und/oder zeitliche Auflösung ist dabei durch das Signal-zu-Rausch Verhältnis (SNR), welches direkt von der Feldstärke des statischen Magnetfeldes abhängt, limitiert. Dabei gilt folgende Relation: je höher $B_0$ desto höher das verfügbare SNR.


Anhand dieses Workflows wurden zwei Spulen entwickelt. Erstens eine $^{31}$P/$^1$H Spule zur Untersuchung von $^{31}$P-metabolischen Vorgängen in der menschlichen Unterschenkelmuskulatur bei gleichzeitiger muskulärer Betätigung. Studienergebnisse, die mit dieser Spule erzielt wurden, werden präsentiert, um die erfolgreiche Realisierung des Workflows zu zeigen. Bei der zweiten Spule handelt es sich um ein $^{31}$P/$^1$H Design zur Untersuchung von $^{31}$P-metabolischen Vorgängen im menschlichen Okzipitallappen bei gleichzeitiger visueller Stimulierung. Vorläufige Ergebnisse dieser Spule sowie mögliche Studiendesigns werden gezeigt.
Publications arising from this thesis

International Peer-Reviewed Journals


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In the past years of my PhD study, I experienced many ups and downs, as do most of us PhD students. Many People, without whom it would most likely not have been possible to finish my PhD, have helped me along the way. This is the moment to express my sincere gratitude to all of the following people.

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Thank you all

"A scientist is a person who knows more and more about less and less, until he knows everything about nothing."

- John Ziman
1.1 General Introduction

Magnetic resonance imaging (MRI) methods are based on the presence of a strong static magnetic field ($B_0$) and the synchronized application of additional time-varying field gradients for spatial encoding as well as a radio frequency (RF) magnetic field ($B_1$) for spin excitation. The required excitation frequency, called Larmor frequency, is directly proportional to $B_0$. The $B_1$ field is traditionally produced by a single "RF-coil", i.e. a conducting structure resonating at the Larmor frequency, generating an RF field orthogonal to the static magnetic field direction. Since the achievable signal-to-noise ratio (SNR) and therefore the potential diagnostic quality of the images is proportional to $B_0$, recent years have seen a constant trend towards higher static field strengths.

Clinically employable MR systems are usually equipped with an RF volume coil (body coil) that is integrated inside the bore [1]. This body coil can be used for transmission and in principle also for reception. However, to increase SNR, frequently smaller receive-only coils positioned closer to the region of interest are used for reception. For higher field strengths ($> 3$ T) the integration of a body coil is not yet possible due to complex RF-body interactions. For the purpose of ultra high field (UHF) MR, transmitting and receiving coils have to be developed, either separately, or combined. Many MR sites focusing on ultra high field MR tend to built their own coils, due to the limited choice of commercially available probes.

The human body mainly consists of water, which has a high relative dielectric permittivity ($\varepsilon_r$) shortening the electromagnetic wavelength ($\lambda$). The additional shortening due to increased frequencies in ultra-high field ($\geq 3$ T) MR lead to highly complex body-RF-field interactions [2]. At 300 MHz, the proton resonance frequency occurring at a $B_0$ of 7 T, the wavelength in tissue is on the order of 13 cm, well below the dimensions of the human body. Consequently, standing wave and wave propagation effects lead to inhomogeneities of the $B_1$ field, which manifest as a modulation of the desired tissue...
contrast and, thus, can severely degrade diagnostic quality. In order to tackle this problem the use of optimized RF coil geometries are required. Another limiting factor of ultra-high field MRI application is power deposition evoked by the concomitant electric field ($E$), measured as the specific absorption rate (SAR). The increasingly inhomogeneous power distribution can lead to focal heating, which can lead to patient burning and has to be avoided at all costs. In order to optimize the performance of the RF coil, the power deposition needs to be considered before the actual assembly.

All these issues can be approached by carefully designing transmitting and receiving probes for the use in UHF MR systems. In order to optimize the geometry of an RF coil and investigate its safety in terms of SAR, its electromagnetic fields inside a realistic human model need to be known. Due to the complexity of the tissue-field interactions, there are no analytical models to calculate the behavior of EM fields inside a realistic human body, thus, numerical full-wave three dimensional electromagnetic simulations (EMS) are required. Most simulations use a discretized model of the RF coil and the sample to calculate the electromagnetic field produced by the RF coil by numerically solving Maxwell’s equations. The method most widely used in the field today is the finite difference time domain (FDTD) method, firstly introduced by Yee in 1966 [3]. FDTD has relatively low hardware requirements and is able to model complex multi-material structures without impact on computation time. Although electromagnetic simulation is a well-established part of RF coil development, real MR methods should also be used to evaluate the accuracy of the simulation. Existing methods for $B_1^+$ mapping and temperature mapping can be employed to achieve high confidentiality in simulation results.

1.2 Outline of the thesis

The main goal of this work was to devise a development workflow for the construction of transmit-receive RF coils for the application in ultra high field MR systems. This workflow identifies the most important steps during construction and should help making the process more efficient for future developments.

After this short introduction, the necessary theoretical background is described in the second chapter which is composed of three main sections. The first section is titled physical theory, including spin dynamics and interaction with a static magnetic field, followed by RF coil design basics, such as RLC electronics, signal acquisition and different probe designs. The basics for numerical simulation with a focus on the finite different time domain method conclude the theory chapter.

The RF coil development workflow is described in detail in chapter three, using the theoretical methods established in chapter two. The workflow is divided into four major steps. First, the preparatory considerations, which define the framework for the future
RF coil, and should give a coarse design notion. This design notion is then investigated with numerical tools in terms of usability, performance and safety, which forms the second step. In the end of step two, an optimized coil design should have been determined. The numerically optimized coil design is built in step three, the bench section. When the coil is physically ready for the use inside the scanner, final tests are conducted inside the MR system. Step four consists of real world tests of the RF probe in terms of safety and performance.

A novel $^{31}\text{P}/^{1}\text{H}$ transceive RF coil for metabolic phosphorus studies in the human calf muscle was developed during this thesis, using the proposed workflow. This work was published in the form of a full paper in *Magnetic Resonance in Medicine* [4]. A complete replica of this publication can be found in chapter four.

Additional studies that were conducted and consequently published are shortly presented in chapter five, while noting that the complete description of these studies would be out of scope of this thesis. I refer the interested reader to the stated citations.

Chapter six presents preliminary results of a novel $^{31}\text{P}/^{1}\text{H}$ RF coil design for phosphorus studies in the occipital lobe at 7 T, again using the developed workflow.

In chapter seven a general conclusion of the thesis is presented. Furthermore, it provides ideas for future developments concerning the presented workflow.
Theoretical Background

2.1 Principles of Magnetic Resonance

In this section the physical principles of nuclear magnetic resonance and its application basics, such as imaging and spectroscopy will be discussed. It is divided into three main parts, starting with the physical background of NMR (2.1.1), followed by the principles used for imaging (2.1.2), and spectroscopy (2.1.3).

There are numerous books that preeminently cover the theoretical foundation of magnetic resonance. The formulas and conclusions discussed within this section, are mainly based on the works of [5, 6, 7, 8], unless stated otherwise.

2.1.1 Physics of Nuclear Magnetic Resonance

2.1.1.1 Nuclear Spin and Magnetic Moment

All elementary particles such as protons, electrons and neutrons possess the fundamental property of an angular momentum called spin \( I \). Spin as a purely quantum mechanical quantity can be assigned not only to sole particles but also to particle assemblies, such as atomic nuclei. Generally spins can be positive or negative, and are of additive nature. Positive spins cancel negative spins, hence a nucleus consisting of multiple particles can possess zero net spin. Only nuclei with an odd atomic mass number will have non-zero net spin. Its magnitude \( |I| \) is quantized and given by

\[
|I| = \hbar \cdot \sqrt{I(I+1)} \quad I = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots \quad (2.1.1)
\]

where \( I \) is called the spin quantum number, and \( \hbar \) denotes the reduced Planck constant.

In classical physics a rotating object with a mass \( m \) has an angular momentum \( \mathbf{L} = \mathbf{r} \times m\mathbf{v} \) (see Fig. 2.1a), where \( \mathbf{v} \) is the velocity at which the object is rotating on an orbit of radius \( r \). If the particle is electrically charged it will constitute a current loop (see Fig. 2.1b).
2. Theoretical Background

![Angular Momentum and Magnetic Moment](image)

**Figure 2.1:** Angular momentum ($L$) and magnetic moment ($\mu$) of a rotating charged particle.

The current produced by this rotating charged particle can be calculated as $i = qf$, where $q$ denotes the charge and $f = \nu / 2\pi r$ the rotation frequency. As a rotating mass with an electric charge it has a magnetic moment ($\mu$) given by

$$\mu = i \cdot A$$  \hspace{1cm} (2.1.2)

where $A = n_A A$ is the vector belonging to the cross-sectional area of the circle it is describing ($A = \pi r^2$).

There exists a relation between angular momentum and magnetic moment denoted by the gyromagnetic ratio $\gamma$:

$$\mu = i \cdot A = \frac{q \nu}{2\pi r} \cdot r^2 \pi \cdot n_A = \frac{q}{2m} \cdot L$$  \hspace{1cm} (2.1.3)

Electrons and protons possess both spin and electric charge, therefore they also have a magnetic moment. Since the spin is a purely quantum-mechanical phenomenon there is no actual rotation and the above relation will yield the wrong result by a dimensionless factor called the g-factor.

In case of an electron the gyromagnetic ratio is given by

$$\gamma_e = \frac{-e}{2m_e} g_e$$  \hspace{1cm} (2.1.4)

where $-e$ is the elementary charge, $m_e$ the electron mass ($= 9.10938291(40) \times 10^{-31}$ [kg]), $\mu_B$ the Bohr magneton ($= 9.27 \times 10^{-24}$ [J/T]), and $g_e$ is the electron g-factor ($= -2.00231930436153(53)$).

Similarly an atomic nucleus consisting of protons and neutrons possesses a net spin. The gyromagnetic ratio for a nucleus is given by

$$\gamma_n = \frac{e}{2m_p} g_{eff}$$  \hspace{1cm} (2.1.5)

where $e$ is the elementary charge, $m_p$ the proton mass ($= 1.6726219 \times 10^{-27}$ [kg]), $\mu_N$ the nuclear magneton ($= 5.0507810 \times 10^{-27}$ [J/T]), and $g_{eff}$ is the effective g-factor.
where $m_p$ is the proton mass ($= 1.672621777(74) \cdot 10^{-27} \text{[kg]}$), $\mu_N$ denotes the nuclear magneton ($= 5.05078353(11) \cdot 10^{-27} \text{[J/T]}$) and $g_{\text{eff}}$ the effective g-factor. Therefore the relation between magnetic moment and spin vector of an arbitrary nucleus can be described with the appropriate gyromagnetic ratio of the associated atom

$$\mu = \gamma_n \cdot I \quad (2.1.6)$$

The following table states the gyromagnetic ratio and spin number for in MRI and MRS commonly used elements:

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>I</th>
<th>$\gamma$ [MHz/T]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1\text{H}$</td>
<td>$1/2$</td>
<td>42.576</td>
</tr>
<tr>
<td>$^{31}\text{P}$</td>
<td>$1/2$</td>
<td>17.235</td>
</tr>
<tr>
<td>$^{13}\text{C}$</td>
<td>$1/2$</td>
<td>10.705</td>
</tr>
<tr>
<td>$^{23}\text{Na}$</td>
<td>$3/2$</td>
<td>11.262</td>
</tr>
</tbody>
</table>

Table 2.1: The gyromagnetic ratio $\gamma$ and spin quantum number $I$ of common NMR relevant nuclei.

2.1.1.2 Spins and Magnetic Fields

In the absence of an external magnetic field the spins are oriented randomly in space. When a magnetic field $B_0$ is applied, the spins align either parallel or antiparallel to it, this is called the Zeeman effect. By convention, the static magnetic field is applied along the z-axis, $B_0 = (0, 0, B_0)$. The component of the net spin vector parallel to the applied magnetic field $I_z$ is quantized and is given by:

$$I_z = \hbar \cdot m_l \quad m_l = -(I - 1), \ldots, (I - 1), I \quad (2.1.7)$$

where $m_l$ denotes the magnetic quantum number with a total of $(2I + 1)$ possible discrete values.

In case of a spin 1/2 system, such as an electron or proton (see Tab. 2.1), there are 2 possible eigenstates for $I_z$:

$$I_z = \begin{cases} +\frac{1}{2}\hbar & \text{I parallel to } B_0 \\ -\frac{1}{2}\hbar & \text{I antiparallel to } B_0 \end{cases} \quad (2.1.8)$$

The potential energy ($E$) of a magnetic moment in the presence of an external magnetic field along $z$ is given by

$$E = -\mu \cdot B_0 = -\gamma I \cdot B_0 = -\gamma I_z B_0 \quad (2.1.9)$$
Therefore when a proton is exposed to an external magnetic field the potential energies of the two eigenstates are

\[ E_{\uparrow, \downarrow} = \pm \frac{1}{2} \hbar \gamma B_0 \]  

(2.1.10)

From the equation above we see that the state parallel to the field direction experiences a lower energy state. The energy difference (\(\Delta E\)) between those states is

\[ \Delta E = \gamma \hbar B_0 \]  

(2.1.11)

The splitting of energy levels in the presence of a magnetic field is called Zeeman splitting (Fig. 2.2a).

![Energy difference](image)

**Figure 2.2**: (a) Energy difference of the two eigenstates of a proton as a function of field strength. The blue arrows indicate the orientation of the spins parallel or antiparallel to the \(B_0\) direction. (b) Spin population difference [ppm] at room temperature (293 K) as a function of field strength (\(B_0\) [T]).

In a system where there is not one isolated particle or nucleus, the distribution of the different spin states follows Boltzmann statistics. In thermal equilibrium the distribution results in a small excess of spins in the lower energy state (\(m_I = +1/2\) see Fig. 2.2a), i.e. aligned with the external magnetic field, giving rise to a net magnetization. The population ratio of the two energy states is given by

\[ \frac{N_\uparrow}{N_\downarrow} = e^{\frac{\Delta E}{k_B T}} = e^{\frac{\gamma \hbar B_0}{k_B T}} \]  

(2.1.12)

where \(k_B\) denotes the Boltzmann constant, and \(N_\uparrow, N_\downarrow\) denote the number of spins aligned with or against the applied field, respectively. At room temperature and for the currently available \(B_0\) field strengths for MRI, the thermal energy \((k_B T)\) is much larger than the magnetic energy \((\gamma \hbar B_0)\), resulting in a very small but detectable net magnetization. The
spin population difference ($\Delta N = N \uparrow - N \downarrow$) can be easily derived from eqn. (2.1.12) in terms of the total spin population ($N_{\text{tot}} = N \uparrow + N \downarrow$):

$$\Delta N = N_{\text{tot}} \left( \frac{e^{\gamma \hbar B_0 / k_B T} - 1}{e^{\gamma \hbar B_0 / k_B T} + 1} \right) = N_{\text{tot}} \cdot \tanh \left( \frac{\gamma \hbar B_0}{2 k_B T} \right) \approx N_{\text{tot}} \cdot \frac{\gamma \hbar B_0}{2 k_B T} \text{ for } k_B T \gg \gamma \hbar B_0 \quad (2.1.13)$$

The population difference at room temperature (293 K) for various magnetic field strengths can be seen in Fig. 2.2b.

The net magnetization of a macroscopic sample is defined as the sum of all magnetic moments within.

$$M = \sum_{n=1}^{N_{\text{tot}}} \mu_n \quad (2.1.14)$$

In thermal equilibrium the Boltzmann distribution of individual spins create a net magnetization along the static $B_0$ field and zero net transverse magnetization due to phase incoherence (see Fig. 2.4a). Substituting equations (2.1.6), (2.1.8) and (2.1.13) into the equation above (2.1.14) gives the following expression for the net magnetization aligned with the applied field,

$$M_0 = \frac{\gamma^2 \hbar^2 B_0 N_{\text{tot}}}{4 k_B T} \quad (2.1.15)$$

The equation above represents the accessible signal in NMR experiments and depends only on the temperature, the static magnetic field strength, and the total number of spins. The inherent low sensitivity of the method, i.e. at room temperature (293 K), and an applied field of 7 T approximately 24 proton spins per million contribute to the signal, is clearly a challenge. In human live samples the temperature is more or less well defined ($\approx 310$ K), as is the spin density per unit volume (for protons $\approx 10^{26} / \text{cm}^3$). Therefore to increase the signal strength one has to increase field strength.

**Spin Precession**

![Spin precession](image)

In classical physics a magnetic moment exposed to a magnetic field $B$ experiences an aligning force called torque $\tau$

$$\tau = \mu \times B \quad (2.1.16)$$

The angular momentum related to the magnetic moment is also related to the torque

$$\frac{dL}{dt} = \tau \quad (2.1.17)$$

This relation holds for spins as well. Using the spin precession representation in Fig. 2.3 the magnitude of the torque is given by

$$|\tau| = \left| \frac{dL}{dt} \right| = I \cdot \sin(\theta) \cdot \left| \frac{d\phi}{dt} \right| = \mu B_0 \cdot \sin(\theta). \quad (2.1.18)$$
Per definition the precession angular velocity is given as the rate of change of the angle \( \varphi \), therefore from eqn. (2.1.18) we get

\[
\omega_L = \frac{d\varphi}{dt} = \frac{\mu B_0 \cdot \sin(\theta)}{I \cdot \sin(\theta)} = \gamma B_0
\] (2.1.19)

This angular precession frequency, at which the magnetic moment precesses about the direction of the magnetic field \( B_0 \), is called the Larmor frequency.

Substituting eqn. (2.1.6) into (2.1.17) and combing it with (2.1.16) yields the equation of motion

\[
\frac{d\mu}{dt} = \gamma \cdot (\mu \times B) = \mu \times \omega_L
\] (2.1.20)

which can be naturally extended to the net magnetization \( M = \sum \mu \):

\[
\frac{dM}{dt} = \gamma \cdot (M \times B) = M \times \omega_L
\] (2.1.21)

The quantum mechanical representation of the NMR phenomenon introduced above, is not very suitable to illustrate the interaction of an ensemble of spins with an external magnetic field. Therefore, from now on, the macroscopic net magnetization vector will be used.

Assuming a static magnetic field along the z-axis \( (B_0) \), the system of differential equations in eq. (2.1.21) breaks down to

\[
\frac{dM_x(t)}{dt} = \gamma B_0 M_y(t)
\] (2.1.22)

\[
\frac{dM_y(t)}{dt} = -\gamma B_0 M_x(t)
\] (2.1.23)

\[
\frac{dM_z(t)}{dt} = 0
\] (2.1.24)

The solution can be easily derived using the relation \( \omega_L = \gamma B_0 \), and choosing the initial condition to be \( M_{x,y,z}(0) = M_{x,y,z}^0 \):

\[
M(t) = \begin{pmatrix}
M_x^0 \cos(\omega_L t) + M_y^0 \sin(\omega_L t) \\
-M_x^0 \sin(\omega_L t) + M_y^0 \cos(\omega_L t) \\
M_z^0
\end{pmatrix}
\] (2.1.25)

This solution states that in the presence of a static magnetic field, the sample magnetization precesses about the \( B_0 \) direction at the Larmor frequency \( \omega_L \).

### 2.1.1.3 Spin Systems and Radio Frequency Fields

Up until now the system investigated was in its equilibrium state (Fig. 2.4a). To be able to detect an NMR signal, the resting state has to be disturbed. Generally, this is achieved
by applying a resonant oscillating magnetic field \((B_1)\) across it. This field, usually in the radio frequency (RF) range, is perpendicular to \(B_0\) and rotates with a frequency equal to the system’s Larmor frequency \(\omega_L\) about the \(z\)-axis. The sample magnetization now precesses about the combined field, and the equation of motion becomes

\[
\frac{dM}{dt} = \gamma \cdot (M \times B) \quad \text{with} \quad B = \begin{pmatrix} B_1 \cos(\omega_L t) \\ B_1 \sin(\omega_L t) \\ B_0 \end{pmatrix}
\]

This precessing motion can be visualized as a *spiraling* motion of the total magnetization vector (Fig. 2.4b). The rotating transverse component of the net magnetization \((M_{xy})\) can be detected, because the changing magnetic field induces a measurable electromotive force \((\xi, \text{emf})\) in a nearby receiver RF coil.

---

**Figure 2.4:** Representation of the initial magnetization due to a static \(B_0\) field. (a) The spins precess about the \(z\) axis according to the equation of motion. Since the phases of the individual spins are randomly distributed (no phase coherence), there is no transverse net magnetization. When a second magnetic field \((B_1)\) is irradiated, the spins start to precess about the combination of both fields, hence the magnetization vector \(M\) follows a spiraling motion (b). In a rotating frame \((B_1)\) along \(\tilde{x}\), this corresponds to the appearance of a net magnetization vector along \(\tilde{y}\) \((M_y)\). On a microscopic level, this can be described as the generation of phase coherence between the individual spins (c).

To visualize this excitation process it is favorable to transform the laboratory frame \((x, y, z)\) into a rotating frame \((\tilde{x}, \tilde{y}, \tilde{z})\), with a rotation frequency equal to \(\omega_L\) (Fig. 2.5a). In the rotating frame, precession about \(B_0\) appears stationary, making the effective static field zero and the magnetization vector of the initial state \((M_0)\) appears constant (Fig. 2.5b and Fig. 2.4a). The additional oscillating RF field is pointing statically in the \(\tilde{x}\) direction and therefore appears constant as well. So in this frame of reference, the magnetization vector only experiences the static \(B_1\) field and will start to precess about
2. Theoretical Background

it, resulting in a simple tilt about $\tilde{x}$ towards the transverse plane (Fig. 2.5c and Fig. 2.4c).

$$B_1 \perp B_0$$

Figure 2.5: The rotating frame (blue) rotates in a clockwise direction around the $z$ axis of the laboratory frame (a). The magnetization vector seen within the rotating frame appears constant (b). When an additional magnetic field is disturbs the system the magnetization vector is tilted about the $\tilde{x}$ axis (c), resulting in a flip angle denoted $\alpha$.

Any linearly polarized field can be decomposed into two circularly polarized counter rotating parts. Only the field rotating in the same direction as the system interacts considerably with the spin system, further on this field will be denoted as the $B_1^+$ or transmit field. The system rotating in the other direction influences the spins in the order of $(B_1/2B_0)^2$, which is known as the Bloch-Siegert shift and is typically very small. This "negatively" rotating field will be denoted as the $B_1^-$ or receive field for reasons explained later on in section ??.

The precessing motion of the spins in the rotating frame corresponds to a flip about the $\tilde{x}$ axis (see Fig. 2.5c). The flip angle produced by an amplitude modulated RF pulse of shape $f(t)$ and duration $\tau$ is given by-

$$\alpha(x) = \gamma B_1^+(x) \int_0^\tau f(t) \, dt$$

This expression simplifies to

$$\alpha = \gamma \tau B_1^+$$

for a rectangular pulse shape. This flip angle depends upon the RF field amplitude and the pulse duration. These excitation pulses can be chosen such that they produce any magnetization flip, e.g. to flip it perpendicular to $B_0$ is called a 90° pulse, while flipping it into an anti-parallel orientation is called 180° pulse.
2.1.4 Relaxation

After the net magnetization of the observed system was tilted into the $xy$ plane by a finitely long RF pulse, the magnetization returns to its equilibrium state. This process is called relaxation. The term actually incorporates two independent relaxation processes, the spin-lattice relaxation, and the spin-spin relaxation, respectively.

Spin-lattice relaxation

The spin-lattice or longitudinal relaxation describes the exponential process of the recovery of $M_z$ after excitation. The rate at which the magnetization vector reverts back to its equilibrium is characterized by a time constant $T_1$. The released energy is deposited in the molecular lattice as the spins realign with the field. This yields the linear differential equation concerning the $z$-component:

$$\frac{dM_z(t)}{dt} = \frac{M_0 - M_z(t)}{T_1} \quad (2.1.29)$$

where $M_0$ denotes the longitudinal magnetization at $t = 0$. The solution to eq. (2.1.29) by simple integration is

$$M_z(t) = M_0 \cdot \left(1 - e^{-\frac{t}{T_1}}\right) \quad (2.1.30)$$

The time constant $T_1$ is also called the longitudinal relaxation time. Figure 2.6 shows the relaxation process where time is measured in multiples of $T_1$.  

\[\text{Figure 2.6: Spin-lattice/longitudinal relaxation process. Some time after the RF pulse excitation the amplitude of the longitudinal magnetization vector is slightly above the initial state (a). The spins are precessing back to their equilibrium state before RF excitation, hence the longitudinal magnetization is increasing (b). This exponential process as a function of time is shown in (c).}\]
Spin-spin relaxation

The second relaxation process is called spin-spin or transverse relaxation. The origin of this phenomenon lies in the spin spin interaction after the initial NMR pulse. While initially the spins perform an in-phase motion, they will soon start to interact with one another, exchanging energy, resulting in local deviations from the Larmor frequency leading to a decay of the net transversal magnetization $M_{xy}$ with a time constant $T_2$. This is described by the differential equations

\[
\frac{dM_x(t)}{dt} = \frac{M_x(t)}{T_2} \quad (2.1.31)
\]
\[
\frac{dM_y(t)}{dt} = \frac{M_y(t)}{T_2} \quad (2.1.32)
\]

which can be as easily solved as eq. (2.1.29) using the rotating frame concept, yielding the solution

\[
M_{xy} = M_{xy}(0) \cdot e^{-\frac{t}{T_2}} \quad (2.1.33)
\]

$T_2$ relaxation times are related to antropy, and are shorter than the corresponding $T_1$ times, which reflect energy exchange. The different values of $T_1$ and $T_2$ times of tissues give rise to contrast in MRI. Table 2.2 states different relaxation times for certain tissues of interest for MRI.

In a real experiment, one will experience a much faster transverse decay than the $T_2$ time predicts. This is due to local inhomogeneities of the $B_0$ field causing additional slight shifts in the local resonant frequency, leading to additional spin dephasing. The time constant predicting this decay is denoted $T_2^*$ and is given by

\[
\frac{1}{T_2^*} = \frac{1}{T_2} + \frac{1}{T_2^*} \quad (2.1.34)
\]
Table 2.2: Characteristic $T_1$ and $T_2$ relaxation times of different tissues at 3 T.

<table>
<thead>
<tr>
<th>Tissue</th>
<th>$T_1$ [ms]</th>
<th>$T_2$ [ms]</th>
</tr>
</thead>
<tbody>
<tr>
<td>gray matter</td>
<td>1300-1500</td>
<td>100</td>
</tr>
<tr>
<td>white matter</td>
<td>900-1000</td>
<td>80</td>
</tr>
<tr>
<td>blood</td>
<td>1550</td>
<td>200-300</td>
</tr>
<tr>
<td>muscle</td>
<td>1100-1400</td>
<td>40</td>
</tr>
<tr>
<td>fat</td>
<td>400</td>
<td>60</td>
</tr>
</tbody>
</table>

where $T_2'$ denotes the influence of local field inhomogeneities, originating mainly from susceptibility differences between different sample tissues, and technical imperfections. The signal loss due to $T_2'$ effects can be recovered by a so called spin echo sequence, which will be introduced in section 2.1.2.4.

**Bloch Equations**

Finally, by including relaxation effects in the equation of motion, leads to the Bloch equations. They fully describe the motion of spins in an external magnetic field under the influence of relaxation processes evoked by a perpendicular time varying RF field:

\[
\begin{align*}
\frac{dM_x}{dt} &= \gamma (M_y B_z - M_z B_y) - \frac{M_x}{T_2} \\
\frac{dM_y}{dt} &= \gamma (M_z B_x - M_x B_z) - \frac{M_y}{T_2} \\
\frac{dM_z}{dt} &= \gamma (M_x B_y - M_y B_x) - \frac{M_z - M_0}{T_1}
\end{align*}
\]  

(2.1.35)

**2.1.1.5 Free Induction Decay**

As shortly mentioned in the previous section, the received signal is the electromotive force ($\xi$) induced in the receive coil via Faraday induction, due to the rotating magnetic field produced by the precessing spins. The course of the induced $\xi$ over time is the NMR signal. Due to the relaxation processes the signal decays after the RF pulse, therefore it is called free induction decay (FID).

**NMR in a nutshell:** Assuming a sample in a static magnetic field, surrounded by an RF coil positioned perpendicular to the static field direction. The RF pulse, oscillating at the Larmor frequency, causes the spins to flip into the transverse plane. When the RF source is switched off the spins start to realign with the main magnetic field and in doing so induce a signal via Faraday induction. This signal is the FID shown in Fig, 2.8.
2. Theoretical Background

2.1.2 Magnetic Resonance Imaging

Exciting the spins (transmission) and acquiring the signal (reception) from a sample volume was explained in the previous section. This methodology can be used to reconstruct images from a sample. To achieve this the signal needs spatial encoding. The foundation of MR imaging, as we know it today, was built in the early 1970’s, where the first magnetic resonance images were obtained using spatial encoding via field gradients [9]. One year later Garroway et al [10] proposed a method for slice selective excitation. The main principles of MRI shall be discussed in the following sections.

2.1.2.1 Fourier Analysis

In general, Fourier analysis may be used to decompose or approximate arbitrary functions by a sum of trigonometric functions. The most widely used technique in Fourier analysis is the Fourier transform. It is a mathematical transform that maps a function in time space to its representation in frequency space. By definition the Fourier transform \( \hat{f} \) of an integrable function \( f : \mathbb{R} \rightarrow \mathbb{C} \) is given by

\[
\hat{f}(\omega) = \int_{-\infty}^{\infty} f(t)e^{-2\pi it\omega} \, dt
\]  

(2.1.36)

A harmonic oscillation in its most basic form, e.g. a sine \( f(t) = \sin(\omega t) \), is characterized by its frequency \( \omega \). Any periodic oscillation can be decomposed into a mixture of harmonic oscillations, differing in frequency and amplitude. The Fourier transform can be used to calculate the frequency spectrum of an arbitrary oscillation. The relationship between time domain and frequency domain can be seen in Fig.2.9.

Using the Fourier transform on the exponentially decaying oscillating FID yields the Larmor frequency of the nucleus of interest (Fig. 2.10). The result is a Lorentzian
2.1. Principles of Magnetic Resonance

Time domain
\[ \sin(\omega_1 t) \]

Frequency domain
\[ \omega_1 \]

\[ \omega_2 \]

Figure 2.9: The time and frequency domain of two periodic oscillations are shown in the figure above. The Fourier transform can be used to switch between these domains.

\[ \sin(\omega_1 t) + a \cdot \sin(\omega_2 t) \]

function, which can be transformed into the FID using the inverse Fourier transform (iFT in Fig. 2.10)

Figure 2.10: The Fourier transform of an FID is a Lorentzian function.

2.1.2.2 Magnetic Field Gradients

Spatial encoding can be achieved by superimposing an additional small, spatially varying magnetic field, increasing linearly from one side to the other, onto the main magnetic field \( B_0 \). This spatial variation will yield a position dependence of the resonance frequency.

Consider the magnetic field \( B_G \) aligned along the \( z \) axis with a spatial variation along \( x \) results in a total magnetic field of

\[ B_{\text{tot}} = (B_0 + B_G \chi) \cdot e_z \] (2.1.37)

where \( B_G \) is constant. This naturally has an influence on the Larmor frequency given by

\[ \omega_L = \gamma (B_0 + B_G \chi) \] (2.1.38)

This can be interpreted as a position dependence of the location along the \( x \) axis of the signal.
Generally the gradient field in MRI can vary along $x$, $y$, and $z$. This magnetic field can be represented as a vector quantity

$$
B_G = \left( \frac{\partial B_z}{\partial x}, \frac{\partial B_z}{\partial y}, \frac{\partial B_z}{\partial z} \right)
$$  \hspace{1cm} (2.1.39)

With this notation, the total magnetic field with a superimposed gradient field described by eq. (2.1.39) is given by

$$
B_{tot}(x) = (B_0 + B_G \cdot x) e_z
$$  \hspace{1cm} (2.1.40)

A typical MRI system today has three independent gradient coils producing field gradients $G_x$, $G_y$, and $G_z$ along the respective axis. Hence, the total gradient field is

$$
B_G = G_x e_x + G_y e_y + G_z e_z
$$  \hspace{1cm} (2.1.41)

In the following paragraphs three methods employing the gradient principle are introduced to achieve signal localization. A combination of the three of them is frequently used in MRI experiments.

**Slice Selection**

The first step in almost any imaging protocol is the slice selection, in order to excite spins in a specific slice of the object. Applying a gradient field along the slice selection axis will yield different precession frequencies of the excited spins (eq. (2.1.38)), and therefore introduces a position dependency. Without loss of generality the $z$-axis is chosen as the slice selection axis, and the gradient will be denoted as $G_{sl}$. This yields the following precession frequency

$$
\omega_L(z) = \omega_0 + \gamma z G_z
$$  \hspace{1cm} (2.1.42)

where $\omega_0$ is the Larmor frequency when there is only the static $B_0$ field present.

When an RF pulse with frequency $\omega_0$ is applied to the system only the spins with Larmor frequency equal to the RF pulse frequency ($\omega_L = \omega_0$) will be excited. Since the Larmor frequency is a function of spatial position this will yield excitation solely in the specified slice. The slice profile in the frequency domain can be determined via Fourier transform of the RF pulse envelope in the time domain, and vice versa. Hence, an infinitely long RF pulse would yield an infinitely thin slice profile (Fig. 2.11a). However, in reality the RF pulse has a finite duration and will contain a band of frequencies, see Fig. 2.11b. So in order to excite a slice in the frequency domain an sinc shaped RF pulse is used.

More formally, the slice position $z_0$ and thickness $\Delta z$ can be determined by

$$
z_0 = \frac{\omega_0 - \gamma B_0}{\gamma G_z}
$$  \hspace{1cm} (2.1.43)

$$
\Delta z = \frac{\Delta \omega}{\gamma G_z}
$$  \hspace{1cm} (2.1.44)
2.1. Principles of Magnetic Resonance

Figure 2.11: The excitation slice profile can be determined as the Fourier transform of the RF pulse shape. Applying an infinitely long RF pulse would result in an infinitely thin slice (a). In reality the RF pulse will not be infinitely long. Applying a sinc pulse would result in a rectangular slice profile (b) and vice versa.

where $\omega_c$ denotes the center frequency and $\Delta \omega$ is the pulse bandwidth. The slice thickness is also dependent on the gradient amplitude $G_z$, therefore a steeper gradient ramp can produce thinner slices. A graphical representation of the slice selection gradient can be seen in Fig. 2.12a

Frequency Encoding

A gradient that is active during the read-out phase, generates a spatial dependence of the precession frequency along the axis it is applied. Without loss of generality the frequency encoding axis shall be the $x$-axis, then the precession frequency becomes a function of the position along $x$. With the help of discrete Fourier transform, the acquired signal can be decomposed into its frequency components, which can then be used to map the signal to its respective spatial location. This method is called frequency encoding, and the gradient is denoted $G_{fr}$.

Phase Encoding

To achieve three dimensional spatial encoding one last gradient is needed. Applying another frequency encoding gradient the signal localization would no longer be fully unique. Therefore, the third method uses the spatially dependent phase information for signal localization, and is called phase encoding method. The phase encoding gradient ($G_{ph}$) is briefly applied along the $y$ axis shortly before the read-out phase. This results in slightly different precession frequencies, depending on the spin’s position along $y$. Then during read-out the phase encoding gradient is switched off, resulting in equal precession frequencies but different phases. Therefore, the phase information can be used to map the position of the spin’s along the $y$ axis.

The three gradient types ($G_{sl}$, $G_{fr}$, $G_{ph}$) constitute the imaging basis for MRI. The use of each gradient and the employed method for signal localization in depicted in Fig. 2.12.
2. Theoretical Background

2.1.2.3 \( k \)-Space

In MRI, the domain in which the images are actually acquired is called \( k \)-space [11]. The normal image space is connected to \( k \)-space via Fourier transform. Following the excitation pulse, the applied gradient waveforms determine the image readout. The readout trajectory that scans the entire \( k \)-space is defined as

\[
k(t) = \gamma \int_0^t G(t') dt'
\]  

(2.1.45)

where \( G = [G_x, G_y, G_z] \) is the applied gradient field, and \( t \) denotes the time following the excitation pulse. The resulting signal time-course is then given as [12]

\[
s(t) = \int_{\text{sample}} \rho(x)e^{-ik(t) \cdot x} dx
\]  

(2.1.46)

where \( \rho(x) \) is the effective spin density distribution at point \( x \). The number of points that are collected along any axis in the \( k \)-space is typically a power of 2, e.g. 64, 128, 256, etc. The coordinates in \( k \)-space represent spatial frequencies, which describe the rate of change of image features with respect to its position (see Fig. 2.13a). Hence, a very homogeneous sample will produce a high amount of low-spatial-frequency signals. High-spatial- frequencies represent a fast change of image feature, which is encountered when different tissue types, or materials meet (see Fig. 2.13b, \( k \)-space images courtesy of [13]).
2.1. Principles of Magnetic Resonance

In the frequency encoding period, k-space data points are sampled along the k-space lines. In the phase encoding period, the location within k-space is altered, resulting in jumps in the trajectory. While applying the phase encoding gradient the signal is not sampled. In order to sample the full image, the full k-space has to be recorded. In reality, only a discrete subset of k-space points can be sampled. An example for a basic Fourier imaging sequence the spin warp sequence [14] is shown in Fig. 2.14. It consists of a slice selective 90° excitation pulse, followed by a phase encoding gradient lobe and frequency encoded readout. The sequence depicted in Fig. 2.14a represents a single k-space line recording. It is repeated in the same manner a number of times to acquire the whole k-space.

2.1.2.4 Imaging Methods

In magnetic resonance imaging the source of the measured signal is usually not the FID shown in Fig. 2.8 but rather an echo. As previously established, the FID signal decays with the time constant $T_2^*$ (see eq. 2.1.34) due to spin dephasing. If the spins are refocused the formed signal is called an echo.

Spin Echo

One way to refocus the spins is by applying a 90° pulse followed by a 180° pulse. The first pulse flips the sample magnetization into the xy plane, where the spins will start to dephase steadily ($T_2^*$ effects), until the measurable signal is 0 although the magnetization has not yet reached its equilibrium state. When a 180° pulse is applied the sign of the dephasing is reversed, resulting in the reformation of a measurable signal (echo).
2. Theoretical Background

Figure 2.14: Spin-warp image sequence. The sequence schematic can be seen in (a), the resulting k-space read out in (b). Each sampling run starts at the k-space center. The first lobe of the frequency and phase encoding gradient, $G_{fr}$ and $G_{ph}$, respectively, moves the readout start away from the center to the left edge. From there the readout gradient, depicted in orange, records the whole k-space line. In the next repetition, the first $G_{fr}$ and $G_{ph}$ lobes move the readout start to another k-space line and samples the respective k-space line. This is repeated until the whole, discrete set of k-space points is recorded.

The method is called spin echo [15] and is depicted in Fig.2.15a. The amplitude of the formed echo is depending on the $T_2$ constant of the nuclei, and therefore yields true $T_2$ contrast.

Gradient Echo

Another possibility of an echo formation uses the gradients to spoil the transverse magnetization, and is therefore called gradient echo method. After applying an RF pulse a linear gradient is applied across the sample forcing the spins to precess differently, depending on the location within the sample. This causes the spins to dephase much faster than the $T_2^*$ effects would cause. Instead of a 180° pulse the gradient field is reversed.
causing the formation of an echo (Fig.2.15b). In terms of contrast, the gradient echo method gives $T_2^*$ contrast. Gradient echoes allow shorter echo times and faster multi-echo sequences. Therefore, 3D-sequences are often GRE based.

### 2.1.3 Magnetic Resonance Spectroscopy

Up until now, the resonance frequency of nuclear spins was said to be dependent on the gyromagnetic ratio and the external magnetic field only (eq. (2.1.19)). In reality, it is also dependent on the chemical environment the nucleus is embedded in. A slight change in frequency, caused by shielding of the nucleus from the magnetic field by surrounding electrons is called chemical shift ($\delta$). The phenomenon which is causing this frequency shift is called electron shielding effect. The electrons behave similarly to protons and neutrons when exposed to an external magnetic field, and start rotating about it in an opposite sense of the proton precession direction. The associated electron magnetic moment acts against the $B_0$ field, resulting in an actual magnetic field ($B_{\text{act}}$) and resonance frequency ($\omega$) given by

$$B_{\text{act}} = B_0(1 - \chi) \quad (2.1.47)$$
$$\omega = \gamma B_0(1 - \chi) \quad (2.1.48)$$

where $\chi$ denotes the dimensionless shielding constant, often expressed in parts per million (ppm). The chemical shift is defined in terms of a reference frequency ($\omega_{\text{ref}}$) of some freely chosen compound:

$$\delta = \frac{\omega - \omega_{\text{ref}}}{\omega_{\text{ref}}} \times 10^6 \quad (2.1.49)$$

where $\omega$ is the resonance frequency of the compound under investigation.

In principle, this chemical shift makes it possible to observe, identify and quantify different metabolites containing NMR.detectable nuclei, such as $^1\text{H}$, $^{13}\text{C}$, $^{31}\text{P}$, and many more. The slightly different Larmor frequencies yield distinguishable signal contributions, therefore we speak of a spectrum. An example proton ($^1\text{H}$) spectrum can be seen in Figure 2.16 courtesy of [6, page 44].

The high spectral resolution achieved by the 11.75 T magnetic field makes it possible to identify 17 different metabolites, which may give information about various biological and/or medical systemic (ab)normalities.

Other examples of elements of interest in modern NMR spectroscopy are

- Phosphorus ($^{31}\text{P}$): to investigate the energy metabolism in cells, as well as intracellular pH concentration, in vivo;
- Carbon ($^{13}\text{C}$): to study metabolic pathways, such as the tricarboxylic acid cycle, in vivo.
Typically, MR RF coils are built to detect signal at the proton resonance frequencies. Due to deviant gyromagnetic constants of different nuclei, the resonance frequency is usually not equal to the proton’s (Tab. 2.1). In order to detect those X-nuclei, specifically built coils, that resonate at the X-nuclei Larmor frequency, are needed. Often a combination of a proton coil together with a X-nucleus coil is used, due to the inherently low sensitivity of most X-nuclei, which makes it difficult to reconstruct a high-resolution image for positioning.

### 2.1.3.1 Phosphorus Spectroscopy

In the work of this thesis, two RF coil arrays were built to detect $^{31}$P metabolites in skeletal muscle and brain (see chapters 4 to 6). To understand the studies that were conducted with both coils, some insight into the role of $^{31}$P in human physiology should be obtained.

Among others, the following biologically relevant $^{31}$P containing metabolites can be detected with $^{31}$P NMR (Tab. 2.3). Those metabolites play a key role in cell energy metabolism, a schematic of which is depicted in Fig. 2.17. Detecting changes in the metabolic concentration can be used for pathological and/or physiological investigations, or to deduce the intracellular pH. Several pathologies have been identified that result from metabolic changes, and therefore, can be detected via $^{31}$P MRS. For example, Stubbs et al. [16] showed the application possibilities in monitoring tumor growth and regression using $^{31}$P MRS. It can also be used for the evaluating the response to targeted cancer cell treatment [17]. In the brain, altered metabolism due to mitochondrial dysfunction has also been observed in early and advanced Parkinson’s [18, 19] and Alzheimer’s disease [20,
2.1. Principles of Magnetic Resonance

Also in psychiatric diseases such as major depression, $^{31}$P MRS can be of diagnostic value [21]. Additional to the application in skeletal muscle examinations, as presented in this work, $^{31}$P NMR contributes to the investigation of cardiac muscle metabolism as well [22]. In all the mentioned application areas, $^{31}$P NMR provides a non-invasive method for investigating the phosphate-rich compounds of cell energy metabolism.

<table>
<thead>
<tr>
<th>Phosphorous containing metabolites</th>
<th>Chemical Shift* [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phosphocreatine (PCr)</td>
<td>0.00</td>
</tr>
<tr>
<td>Inorganic phosphate (Pi)</td>
<td>5.02</td>
</tr>
<tr>
<td><strong>Adenosine diphosphate (ADP)</strong></td>
<td></td>
</tr>
<tr>
<td>$\alpha$</td>
<td>-7.05</td>
</tr>
<tr>
<td>$\beta$</td>
<td>-3.09</td>
</tr>
<tr>
<td><strong>Adenosine triphosphate (ATP)</strong></td>
<td></td>
</tr>
<tr>
<td>$\alpha$</td>
<td>-7.52</td>
</tr>
<tr>
<td>$\beta$</td>
<td>-16.26</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>-2.48</td>
</tr>
<tr>
<td><strong>Phosphomonoesters (PME)</strong></td>
<td></td>
</tr>
<tr>
<td>Phosphorylethanolamine</td>
<td>6.78</td>
</tr>
<tr>
<td>Phosphorylcholine</td>
<td>5.88</td>
</tr>
<tr>
<td><strong>Phosphodiesters (PDE)</strong></td>
<td></td>
</tr>
<tr>
<td>Glycerol-3-phosphorylethanolamine</td>
<td>3.20</td>
</tr>
<tr>
<td>Glycerol-3-phosphorylcholine</td>
<td>2.76</td>
</tr>
</tbody>
</table>

* (relative to PCr)

Table 2.3: Biologically relevant and MRS detectable phosphorous metabolites.

Figure 2.17: The energy provision mechanisms in skeletal muscle during exercise are depicted in this figure. The three main metabolic pathways of ATP generation include (a) the ATP-PCR (ATP-phosphagen) system as described above, (b) the anaerobic glycolysis and (c) the oxidative phosphorylation in mitochondria. Figure by courtesy of [23].
Adenosine triphosphate (ATP) and Adenosine diphosphate (ADP): ATP acts as an energy source in biological cell metabolism. A molecule of ATP contains three phosphate groups. When one group is donated to produce energy, the resulting molecule has two phosphate groups left and is therefore called Adenosine diphosphate (ADP). There are various ways how the organism produces ATP, i.e. by oxidative phosphorylation in the mitochondria (Fig. 2.17c), glycolysis (Fig. 2.17b) or the ATP-phosphagen system (Fig. 2.17a). Normal ATP concentration in the brain varies for gray ($\approx 2 \text{ mM}$) and white matter ($\approx 3.5 \text{ mM}$), whereas in skeletal muscle it is $\approx 6.8 \text{ mM}$ [6, 24]. This amount of ATP would allow the cell a few seconds of high energy actions [25]. Therefore human cells tend to store phosphorylated creatine (PCr) as an energy buffer.

Phosphocreatine (PCr) and inorganic phosphate (Pi): One possible metabolic pathway of ATP generation during intense activity is the ATP-phosphagen system. Within that system PCr is degraded to creatin (CR) by a creatine kinase (CK) to produce free Cr and Pi. The free Pi is donated to ADP to form ATP by an ATPase. PCr is therefore often described as a high-energy phosphate reserve. During rest, excessive ATP can be used to reform PCr from free Cr. Therefore PCr is mainly found in tissues with high energy fluctuations, such as muscle, and brain. Normal PCr concentration in the human brain is 4.0-5.5 mM [6], whereas in skeletal muscle the concentration is much higher $\approx 33 \text{ mM}$ [24].

An example $^{31}\text{P}$ spectrum of a rat skeletal muscle can be seen in Fig. 2.18a, showing the described PCr, Pi, and ATP peaks.

Figure 2.18: (a) The $^{31}\text{P}$ spectrum originating from rat skeletal muscle is shown. Visible metabolites are inorganic phosphate (Pi), phosphocreatine (PCr), and ATP $\alpha$, $\beta$, $\gamma$ each corresponding to a phosphate group in ATP. The spectrum is by courtesy of [6, page 79]. (b) Calculation of the pH shift in terms of the Pi shift towards/away from the PCr peak.
The exact chemical shift of $^{31}$P-containing metabolites may vary depending on the intracellular pH and magnesium concentration. This is caused by a change of the chemical environment of a nucleus due to protonation of a nearby compound, and results in a slightly different chemical shift/resonance frequency. Since the resonance frequency is now dependent on the relative amount of protonated and unprotonated forms, the intracellular pH can be calculated in terms of the observed chemical shift ($\delta$), and the protonated ($\delta_{HA}$) and unprotonated ($\delta_{A}$) chemical shift of some compound A [6]:

$$\text{pH} = \text{pK}_A + \log\left(\frac{\delta - \delta_{HA}}{\delta_{A} - \delta}\right)$$

(2.1.50)

where $\text{pK}_A$ is the logarithm of the equilibrium constant for the acid–base equilibrium between $HA$ and $A$.

This pH dependency can be readily observed in inorganic phosphate (Pi). In the physiological pH range the $PCr$ peak is assumed constant. If there is a change in intracellular pH the $Pi$ peak shifts towards or away from the $PCr$ peak (see Fig. 2.18b) depending on whether the change is alkaline or acidic.
2.2 Radio Frequency Coil Design

The radio frequency (RF) coil in an NMR experiment is used to transmit an electromagnetic field, perpendicular to the main magnetic field $B_0$, at a frequency equal to the Larmor frequency of the nuclei of interest, and to receive the signal as an induced electromotive force by the magnetic field generated by the excited spins precessing back to equilibrium. Simply put, the RF coil acts as a connection between the sample and the MR system.

In general, an RF coil is able to perform the transmit and receive part of an NMR experiment, such coils are called "Transceivers". There is also the possibility of separating the transmitting and receiving coil. In this case, which is the more commonly used in MRI, the receive coil has to be detuned during transmission, as not to disturb the excitation. Most MR systems at and below 3 T have a big transmit coil incorporated into the scanner called body coil. This has the advantage that the transmitting part has to be not considered for coil development.

2.2.1 Transmission and Reception

As previously addressed in section 2.1.1.3, only one circularly polarized field is influencing the spins, namely the one that is rotating in the same sense as the precessing spins. This transmission field is denoted $B_1^+$, regardless of what the actual sense of rotation is.

Decomposition of the $B_1$ field to polarized components

Any linearly polarized field can be decomposed into two counter rotating components, which can be seen in Fig. 2.19a.

![Decomposition into circularly polarized fields](image)

**Figure 2.19**: (a) depicts the decomposition into two (clockwise and counter-clockwise) counter rotating circularly polarized fields with frequencies $\omega t$. (b) shows the projection of the x and y field components onto the rotating frame.
2. Theoretical Background

The magnetic field produced by the RF coil (B₁) can easily be resolved into its vector components \([B_{1x}, B_{1y}, B_{1z}]\), which are generally oscillating at the same frequency and phase. However, due to displacement and conduction currents at high frequencies, the calculation of the vector components get somehow more complex. The \(B_0\) field is assumed to be aligned along \(z\), therefore neglecting the \(z\) components, the \(x\) and \(y\) field components can be written as [26]:

\[
B_{1x} = \hat{B}_{1x} \cos(\omega t + \varphi + \alpha) \tag{2.2.1}
\]

\[
B_{1y} = \hat{B}_{1y} \cos(\omega t + \varphi + \beta) \tag{2.2.2}
\]

Here, \(\hat{B}_{1x,1y}\) are the position and frequency dependent amplitudes of the field components, while \(\alpha\) and \(\beta\) are position and frequency dependent changes of phase due to the mentioned displacement and conduction currents.

We are now interested in the \(B_1\) field produced when we work in the rotating frame \((\hat{x}, \hat{y}, \hat{z})\). Assuming the positively rotating frame rotates at a frequency of \(\omega\), then at time point \(t\) the rotating frame makes an angle of \(\omega t\) with the laboratory frame (see Fig. 2.19b). By simple projection we can write the field components of the \(B_1\) field in the rotating frame:

\[
\hat{B}_{1x}^{(+)} = B_{1x} \cos(\omega t) + B_{1y} \sin(\omega t) \tag{2.2.3}
\]

\[
\hat{B}_{1y}^{(+)} = -B_{1x} \sin(\omega t) + B_{1y} \cos(\omega t) \tag{2.2.4}
\]

The superscript \(^{(+)}\) symbolizes that we are operating in the positively (\(+\omega t\)) rotating frame, for the negatively (\(-\omega t\)) rotating frame a similar expression can be found. Substituting eqn. (2.2.1), and (2.2.2) into (2.2.3) and (2.2.4), the resulting products of cosine and sine lead to terms with no time dependency, and terms with time variations of \(2\omega t\). The \(2\omega t\)-terms can be neglected, since they are not influencing the NMR signal. This yields the following expressions:

\[
\hat{B}_{1x}^{(+)} \approx \frac{1}{2} \left[ \hat{B}_{1x} \cos(\varphi + \alpha) - \hat{B}_{1y} \sin(\varphi + \beta) \right] \tag{2.2.5}
\]

\[
\hat{B}_{1y}^{(+)} \approx \frac{1}{2} \left[ \hat{B}_{1x} \sin(\varphi + \alpha) + \hat{B}_{1y} \cos(\varphi + \beta) \right] \tag{2.2.6}
\]

For reasons of simplicity, it is worth taking a digression into the complex number notation. In the following, complex quantities are underlined. The \(x\) and \(y\) field components in the laboratory frame are then the real part of a complex quantity defined by

\[
B_{1x} = \text{Re}(\hat{B}_{1x}e^{i\omega t}); \quad B_{1x}^{\dagger} = \hat{B}_{1x}e^{i(\varphi + \alpha)} \tag{2.2.7}
\]

\[
B_{1y} = \text{Re}(\hat{B}_{1y}e^{i\omega t}); \quad B_{1y}^{\dagger} = \hat{B}_{1x}e^{i(\varphi + \beta)} \tag{2.2.8}
\]
2.2. Radio Frequency Coil Design

For the components in the laboratory frame, we can rewrite eqn. (2.2.5) and (2.2.5) into the following form

\[
\begin{align*}
\vec{B}_{1x}^{(+)} &= \frac{1}{2} \text{Re}(\vec{B}_{1x} + i\vec{B}_{1y}) \\
\vec{B}_{1y}^{(+)} &= \frac{1}{2} \text{Re}(-i\vec{B}_{1x} + \vec{B}_{1y}) = \frac{1}{2} \text{Im}(\vec{B}_{1x} + i\vec{B}_{1y})
\end{align*}
\] (2.2.9, 2.2.10)

In the equations above, we have the real and the imaginary part of the same expression. We will use the Argand diagram, i.e. real numbers are along \( \vec{x} \) while imaginary numbers are along \( \vec{y} \), for expressing the \( \vec{B}_1 \) field in the rotating frame:

\[
\vec{B}_1^{(+)} = \vec{B}_{1x}^{(+)} + i\vec{B}_{1y}^{(+)} = \vec{B}_{1x} + i\vec{B}_{1y}
\] (2.2.11)

Similar considerations lead to the following expression for the \( \vec{B}_1 \) field in the negatively rotating frame [26]:

\[
\vec{B}_1^{(-)} = \vec{B}_{1x}^{(-)} + i\vec{B}_{1y}^{(-)} = \frac{(\vec{B}_{1x} - i\vec{B}_{1y})^*}{2}
\] (2.2.12)

where the asterisk denotes the complex conjugate. This definition of the transmit (\( \vec{B}_1^+ \)) and receive (\( \vec{B}_1^- \)) field is used throughout this thesis without the underline.

### 2.2.1.1 Principle of Reciprocity

The magnetic field that is generated by a transmitter coil is produced via current passing through the RF coil. Using Ampère’s law this can be described as

\[
\oint_C \vec{B} \, d\ell = \mu_0 \int_S \vec{J} \cdot d\vec{S}
\] (2.2.13)

where \( C \) is a closed curve, \( S \) is the surface bounded by \( C \), and \( \vec{J} \) is the current density.

After excitation the spins precess back to equilibrium, and in doing so produce a rotating magnetic field which induces an electromagnetic force (\( \xi \)) in the receive RF coil. This is described by Faraday’s law of induction:

\[
\xi = -\frac{d\Phi}{dt} = -\frac{d}{dt} \int_S \vec{B} \cdot d\vec{S}
\] (2.2.14)

where \( \Phi \) denotes the magnetic flux.

The principle of reciprocity forms a bridge between transmit field and receive sensitivity of an RF coil. It states that the signal induced in a receive coil by the precessing spins is proportional to the hypothetical field produced by the coil when applying unit current [26].

The magnetic field produced by moving charges in the coil can be defined using the vector potential \( \vec{A} \) such that

\[
\vec{B} = \nabla \times \vec{A}
\] (2.2.15)
2. Theoretical Background

where \( \mathbf{A} \) at position \( \mathbf{r} \) can be derived from the solution of Poisson’s equation as a Green’s function \[8\]

\[
\mathbf{A}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int_V d^3r' \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}
\]

(2.2.16)

In the equation above, \( \mathbf{J}(\mathbf{r}) \) denotes the current density at position \( \mathbf{r} \). With the help of the product rule for scalar and vector functions \( [\nabla \times (\partial \mathbf{A}) = \partial \nabla \times \mathbf{A} + \nabla \partial \times \mathbf{A}] \), the magnetic field produced by the RF coil can be calculated as

\[
\mathbf{B}_1(\mathbf{r}) = \nabla \times \mathbf{A} = -\frac{\mu_0}{4\pi} \int_V dV' \mathbf{J}(\mathbf{r}') \times \nabla_r \left( \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right)
\]

(2.2.17)

where \( \nabla_r \) denotes that the curl operations are acting on \( \mathbf{r} \) rather than on \( \mathbf{r}' \). Now replacing the integration of the current density over the whole volume by the integration of the current \( I \) in the coil yields Biot-Savart’s law

\[
\mathbf{B}_1(\mathbf{r}) = -\frac{\mu_0 I}{4\pi} \oint_C dl \times \nabla_r \left( \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right)
\]

(2.2.18)

The magnetic flux \( \Phi \) through the surface \( S \) is defined by

\[
\Phi = \iint_S \mathbf{B} \cdot d\mathbf{S} = \iint_S \nabla \times \mathbf{A} \cdot d\mathbf{S} \equiv \oint_{\partial S} \mathbf{A} \cdot dl
\]

(2.2.19)

using the classical Kelvin–Stokes (KS) theorem. The contribution of the net magnetization to the current density at a specific point in the sample \( \mathbf{r} \) at time \( t \) is given by

\[
\mathbf{J}(\mathbf{r}, t) = \nabla \times \mathbf{M}(\mathbf{r}, t)
\]

(2.2.20)

Using eq. (2.2.16), the vector potential produced by the net magnetization in the sample at position \( \mathbf{r} \) and time \( t \) in the coil wire therefore is

\[
\mathbf{A}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \int_V d^3r' \nabla \times \mathbf{M}(\mathbf{r}, t) = -\frac{\mu_0}{4\pi} \int_V \mathbf{M}(\mathbf{r}', t) \times \nabla_r' \left( \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) dV'
\]

(2.2.21)

This expression can be inserted into eq. (2.2.19) yielding the following expression for the magnetic flux

\[
\Phi = -\oint_C \left[ \frac{\mu_0}{4\pi} \int_V \mathbf{M}(\mathbf{r}', t) \times \nabla_r' \left( \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) dV' \right] \cdot dl
\]

(2.2.22)

which can be rearranged using the vector identity \( [(\mathbf{A} \times \mathbf{B}) \cdot \mathbf{C} = -\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C})] \):

\[
\Phi = \int_V \mathbf{M}(\mathbf{r}', t) \cdot \frac{\mu_0}{4\pi} \oint_C dl \times \nabla_r' \left( \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right) dV'
\]

(2.2.23)

Back to Faraday’s induction (2.2.14). The electromotive force is defined as the rate of change of the magnetic flux

\[
\xi(t) = -\frac{d\Phi(t)}{dt} \equiv -\frac{d}{dt} \int_V \mathbf{M}(\mathbf{r}', t) \cdot \mathbf{B}_1(\mathbf{r}') \cdot dV'
\]

(2.2.24)
where $\mathbf{B}_1(r')$ is the magnetic field of a coil driven with unit current. This key formula shows the dependence of the voltage induced in the receive coil on the $\mathbf{B}_1$ field that it would produce as a transmit coil per unit current. This is called the principle of reciprocity. It allows the assessment of the signal strength received in a coil by considering it’s theoretic transmit field.

### 2.2.2 Signal and Noise in MR

The signal obtained by an MR experiment contains additional noise superimposed on the original signal. The signal-to-noise-ratio (SNR) determines the limit of signal detection in an MR experiment. It is defined as the ratio of the electromotive force induced in the RF coil over the noise voltage. To avoid additional noise sources due to external RF signals, the scanner is usually placed in a Faraday cage.

The signal can be described using the principle of reciprocity described in the previous section. Assuming a homogeneous $\mathbf{B}_1$ field within a voxel, which is valid for the usually used voxel sizes in MR, eq. (2.2.24) becomes

$$\mathcal{E}_i = \omega_0 B_{1,xy} M_0 V \cos(\omega_0 t)$$

(2.2.25)

where $B_{1,xy}$ is the transverse component of the receptive $B_{1}^{-}$ field. Remembering the $B_0$ proportionality to $\omega_0$ and $M_0$ it follows that the signal amplitude is proportional to the square of the main magnetic field strength,

$$\mathcal{E} \propto B_0^2$$

(2.2.26)

The noise voltage can be derived using the fluctuation dissipation theorem, which states that the noise sources are driven by thermal excitation of electric charges in electrical conductors. This was observed by Nyquist in 1928 [27] and put into the following equation:

$$V_{\text{noise}} = \sqrt{4k_B T \Delta f R}$$

(2.2.27)

where $V_{\text{noise}}$ denotes the produced RMS voltage, $k_B$ is the Boltzmann constant, $T$ is the absolute temperature, $\Delta f$ is the receiver bandwidth, and $R$ denotes the equivalent total noise resistance as seen from the output terminals.

Nyquist’s equation shows another relation between transmit and receive performance of a coil. Each dissipative loss mechanism during transmit, i.e. ohmic resistances, represents a noise mechanism during reception. The equivalent resistance ($R$) is constituted of two noise sources, the coil resistance ($R_c$) and sample resistance ($R_s$). The coil resistance is a result of ohmic losses within the coil’s material. Due to the tendency of an alternating current to have a larger current density close to the surface (skin effect), the coil resistance is increased at higher frequencies. This yields the following relation [28]

$$R_c \propto \sqrt{\omega_0} \propto \sqrt{B_0}$$

(2.2.28)
Coil losses are minimized using good conductors (e.g. copper) and careful soldering.

The main sample noise contribution results from magnetically coupled noise. Induced eddy currents and thermally agitated electric charges generate a voltage in the receive coil that cannot be distinguished from the signal voltage. This results in a random fluctuation of the MR signal. The noise generated by magnetic coupling is not affected by increasing field strength, but the sample coupling increases linearly with frequency. Therefore the following relationship between sample noise and $B_0$ can be established [29, 30]:

$$R_s \propto \frac{V_{\text{noise},s}}{\sqrt{B_0}} \propto B_0^2$$ \hspace{1cm} (2.2.29)

Magnetic interactions with the sample cannot be avoided since it is necessary for signal generation. Nevertheless, avoiding coil interaction with other structures than the ROI is advised.

Using eqn. (2.2.26) to (2.2.29) yields the following relationship,

$$\text{SNR} = \frac{\xi}{V_{\text{noise}}} = \frac{\omega_0 B_0^{-1} M_0 V \cos(\omega_0 t)}{\sqrt{4kT \Delta f R}} \propto \frac{B_0^2}{\sqrt{B_0^2 + \alpha \sqrt{B_0}}}$$ \hspace{1cm} (2.2.30)

where $\alpha$ depends on the ratio of $R_s$ to $R_c$, and can be used to establish the coil noise and sample noise domains. At low frequencies, or small sample/coil sizes, coil noise is the dominating source, yielding an SNR dependency of $\frac{1}{\sqrt{B_0^2}}$. Whereas, when sample noise is dominating, the SNR dependency is proportional to $B_0$.

In typical MR experiments the sample noise is the dominating noise source, hence $\text{SNR} \propto B_0$. Sophisticated coil design can be used to minimize sample noise, e.g. coil miniaturization. If for some reason the coil noise is the dominating factor, the RF probe design can be adapted to decrease the coil resistance, e.g. cooling the coil.

### 2.2.2.1 Coil Efficiency

The coil transmit efficiency ($\eta$) can be defined as the ratio of the effective power density delivered to a point in space ($|B_t|^2$) to the total power absorbed in the target region ($P_{\text{abs}}$) [31]:

$$\eta = \frac{|B_t|^2}{\frac{1}{2}|I|^2 R}$$ \hspace{1cm} (2.2.31)

Setting the input current to 1 A and using the principle of reciprocity, a connection between eq. (2.2.30) and (2.2.31) is established,

$$\text{SNR}^2 \propto \eta = \frac{|B_t|^2}{P_{\text{abs}}}$$ \hspace{1cm} (2.2.32)

This equation provides a link between the coil efficiency as a transmitter and the signal-to-noise ratio it produces as a receiver. This formulation is especially useful when comparing different coil designs.
2.2.3 RLC circuits

The RF coil in its most basic function, is an electrical device that is designed to create, and/or be sensitive to a magnetic field. It usually consists of an inductance (\(L\)), i.e. the copper wire of the coil, at least one capacitance (\(C\)), and naturally also a resistance (\(R\)) concomitant to the inductance. Therefore, this electrical device can be represented as a resonant RLC circuit (Fig. 2.20).

\[
\begin{align*}
\text{(a) Series RLC configuration} & & \text{(b) Parallel RLC configuration} \\
\end{align*}
\]

**Figure 2.20:** (a) shows a simple representation of an RF coil as a series RLC circuit, a loop consisting of copper wire (\(L\)) with a series capacitance (\(C\)). In the appropriate equivalent circuit the concomitant resistance of the copper wire is shown in series to \(L\). (b) depicts the RF coil representation as a parallel RLC circuit, with one capacitance in series (\(C_t\)) and one in parallel (\(C_{tm}\)), and its equivalent circuit.

An important property of RLC circuits and their electrical elements is their impedance (\(Z\)). The impedance of an alternating current (AC) circuit can be regarded as a concept extension of a resistance of a direct current (DC) circuit. It is a complex entity and, therefore, possesses magnitude and phase, and can be written as

\[
Z = R + iX
\]  \hspace{1cm} (2.2.33)

where the real part \(R\) is called resistance, and the imaginary party \(X\) is called reactance, both are measured in ohm. The impedance of an electrical element describes the relation between current and voltage using Ohm’s law

\[
Z = \frac{V}{I}
\]  \hspace{1cm} (2.2.34)

The voltage across an inductor is given by [7]

\[
V = L \frac{dI}{dt}
\]  \hspace{1cm} (2.2.35)

where \(L\) denotes the inductance, and \(I\) denotes the current. If we assume the current to be \(I = I_0 \cos(\omega t)\), then the voltage across the inductor is

\[
V = -L I_0 \omega \sin(\omega t) = X_L I_0 \cos(\omega t + 90^\circ)
\]  \hspace{1cm} (2.2.36)
where $\omega$ is the angular frequency. Hence, the phase of the voltage across an inductor advances that of the current about $+90^\circ$, and its amplitude is proportional to $X_L = \omega L$, and is called inductive reactance.

Now the dissipated power can be calculated as the product of voltage and current ($W = IV$), and in case of an inductor is

$$W = -\frac{1}{2} I_0^2 \omega L \sin(2\omega t) \quad (2.2.37)$$

which is zero on average. This shows that there is no power dissipated in a pure inductor.

A very similar relationship of voltage and current can be deduced for a capacitor, with the difference that now the phase difference between current and voltage is $-90^\circ$ and the amplitude is proportional to $X_C = -1/\omega C$ (capacitive reactance), which is the reactance of the capacitor, and again no power is dissipated in a capacitor.

The only electrical element which dissipates power is the resistance ($R$). There is no phase change between current and voltage and therefore the dissipated power is $W = IV = I_0^2 R \cos(\omega t)$, which on average is

$$W = \frac{1}{2} I_0^2 R \quad (2.2.38)$$

These properties are summarized in Tab. 2.4.

<table>
<thead>
<tr>
<th>Phase difference of current vs. voltage</th>
<th>Impedance $Z \ [\Omega]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resistance ($R$)</td>
<td>$0^\circ$</td>
</tr>
<tr>
<td>Inductance ($L$)</td>
<td>$+90^\circ$</td>
</tr>
<tr>
<td>Capacitance ($C$)</td>
<td>$-90^\circ$</td>
</tr>
</tbody>
</table>

**Table 2.4:** Phase relation for voltages and current through resistance, inductance, and capacitance and their impedance. The impedance of a pure capacitor and inductor is the reactance, it is an imaginary entity, hence the imaginary unit $i$ in the formulas above.

To determine the total impedance of a circuit consisting of parallel and/or series impedances the following two rules apply.

For a series impedance circuit the resulting total impedance can be calculated as

$$Z_{AB} = Z_1 + Z_2 + .. + Z_n \quad (2.2.39)$$

For a parallel impedance circuit the total impedance can be calculated as

$$\frac{1}{Z_{AB}} = \frac{1}{Z_1} + \frac{1}{Z_2} + .. + \frac{1}{Z_n} \quad (2.2.40)$$
2.2.3.1 Resonance

For reasons that should be clear after reading the following sections, RF coils are usually resonant structures. Determining its resonance frequency and equating it to the needed Larmor frequency of the system is a process called tuning. The natural frequency of LC circuits can be derived with the help of Kirchhoff’s voltage and current laws [32], and happens when the inductive reactance equals the capacitive reactance, and the imaginary part of the circuits impedance is zero

\[ \omega_0 = \frac{1}{\sqrt{LC}} \quad (2.2.41) \]

This can be seen as a constant exchange of energy between capacitor and inductor at each cycle, and a very slow dissipation of energy solely in the pure resistance of the circuit. The resonance frequency of s series RLC circuit as described in Fig. 2.20a equals the natural frequency \( \omega_r = \omega_0 \).

In case of the parallel resonant circuit shown in Fig. 2.20b, the total impedance can be expressed using Tab. 2.4, eq. (2.2.39) and (2.2.40) as

\[ \frac{1}{Z_{\text{tot}}} = \frac{1}{R + i\omega L} + i\omega C \quad (2.2.42) \]

The real and imaginary part of the total impedance are given as

\[ \text{Re}(Z_{\text{tot}}) = \frac{R \cdot (L\omega)^2}{R^2 + (L\omega - \frac{1}{C\omega})^2} \]

\[ \text{Im}(Z_{\text{tot}}) = -\frac{1}{C\omega} \cdot \frac{R^2 + L\omega(L\omega - \frac{1}{C\omega})}{R^2 + (L\omega - \frac{1}{C\omega})^2} \]

The imaginary part cancels at a frequency very close to the natural frequency \( \omega_0 \) when

\[ R^2 + L\omega(L\omega - \frac{1}{C\omega}) = 0 \quad (2.2.43) \]

namely at the frequency

\[ \omega_r = \sqrt{\frac{1}{LC} - \frac{R^2}{L^2}} \quad (2.2.44) \]

This resonance frequency is very close to the natural frequency since usually \( R << L \).
Since in NMR a very specific resonance frequency is needed, namely the Larmor frequency, the coil’s resonance has to be adjusted to meet that requirement. This can be done by altering either the inductance or the capacitance. The inductance and the resistance are determined by the coil geometry, which on the other hand is determined by the application area, and can usually not be changed. Therefore it is common practice to change the capacitance of the coil to reach the desired frequency.

### 2.2.3.2 Impedance Matching

In order to use the RF coil for NMR experiments tuning alone is not sufficient. The coil needs to be connected to preamplifiers, switches, and the scanner’s RF chain. All of these components are designed to work at an arbitrarily chosen characteristic impedance, most commonly 50 $\Omega$. The impedance seen at the RF coil’s port is most likely not equal to this characteristic impedance. To ensure efficient power transfer, the coil impedance has to be transformed.

![Impedance as a function of frequency for a parallel resonant circuit](image)

**Figure 2.22:** Impedance as a function of frequency for a parallel resonant circuit. On resonance the reactance is zero and the resistance is at a maximum at $QL\omega_0$. At two frequencies off resonance ($\omega_1, \omega_2$) the resistance exactly equals 50 $\Omega$.

The impedance of a parallel resonant circuit (Fig. 2.20b) is frequency dependent. A representation of the real and imaginary part of $Z$ around its resonance frequency ($\omega$) can be seen in Fig. 2.22. At the resonance frequency the reactance equals zero and the resistance of the circuit is at a maximum ($QL\omega$), usually not equal to 50 $\Omega$. However, at two frequencies slightly off resonance ($\omega_1, \omega_2$) the desired resistive 50 $\Omega$ plus some reactive part is reached.
The reactance at those frequencies can easily be canceled using a series capacitance or inductance, although the capacitive matching (Fig. 2.23) is more favorable since the concomitant resistance is much smaller than with an inductance. The tuning capacitors \( C_t \) and \( C_{tm} \) can be adjusted to make \( \omega_1 \) or \( \omega_2 \) the Larmor frequency.

![Figure 2.23: A simple representation of an tuned and matched RF coil. The parallel and series capacitors \( C_{tm} \) and \( C_t \) are used to tune the coil to the Larmor frequency and the series capacitor \( C_m \) is used to match the coil to 50 \( \Omega \).](image)

In realistic coil models several capacitors are placed in series to yield a more even current distribution, and reduce the electric field by the probe.

### 2.2.4 Q-factor

Generally, the Q-factor of a resonator is defined as the energy stored to the energy dissipated per cycle. This translates to the ratio of reactance to resistance for RLC circuits:

\[
Q = 2\pi \cdot \frac{\text{energy stored}}{\text{energy dissipated per cycle}} = \frac{X}{R} \tag{2.2.45}
\]

In case of an RF coil, where \( \omega L >> 1/\omega C \), this simplifies further to

\[
Q = \frac{\omega L}{R} \tag{2.2.46}
\]

Another, probably more common definition of the Q-factor is the frequency-to-bandwidth ratio given by

\[
Q = \frac{\omega_0}{\Delta \omega} \tag{2.2.47}
\]

where \( \omega_0 \) is the resonance frequency, and \( \Delta \omega \) is the -3 dB (half power) bandwidth. The definitions are equivalent for high Q values, which can be seen in [33].

When a sample is placed close to the coil, the resistance seen at the coil port, increases, since tissue mass consists of conducting, lossy materials magnetically coupled to the RF coil. The Q-factor then is given by:

\[
Q_t = \frac{\omega L}{R_c + R_s} \tag{2.2.48}
\]
2. Theoretical Background

where $R_c$ is the ohmic resistance in the coil structure, and $R_s$ is the resistance in the sample. Usually $R_s$ is much bigger than $R_c$, therefore, the coil resistance can be neglected. How much bigger $R_s$ is strongly depends on the coil size. When the coil is getting smaller, also the induced sample resistance decreases. Once $R_c > R_s$, the coil resistance is the main source of noise and can be reduced, e.g. by using cooled or superconducting coils. Therefore, it is useful to look at the ratio of unloaded ($Q_u$) vs. loaded $Q$ ($Q_l$).

$$Q_{\text{ratio}} = \frac{Q_u}{Q_l} = \begin{cases} \in [2, \infty[ & R_s \geq R_c \\ \in [1, 2[ & R_s < R_c \end{cases} \quad (2.2.49)$$

A Q-ratio of 2 and above indicates sample noise dominance, which is the regime most MR coils are operating in.

2.2.5 Specific Absorption Rate

Generally, an oscillating magnetic field comes along with an oscillating electric field that causes conduction currents in surrounding tissue, resulting in deposited power, and inducing electromagnetic fields that will further propagate into the tissue. The specific absorption rate (SAR) is a measure for the absorbed energy in the sample, e.g. the human body, when exposed to an electromagnetic field. The RF energy dissipated in tissue sample results in heating [34], which may harm the patient. The SAR value is defined as the ratio of total RF energy dissipated in the sample over the exposed sample mass. The dissipated power in a sample volume ($V$) can be derived from Poynting’s theorem [35]:

$$P_{\text{abs}} = \int_V \frac{\sigma(x) |E(x)|^2}{2} \, dx \quad (2.2.50)$$

where $\sigma$ denotes the electrical conductivity in the sample, and $E$ is the electric field. The SAR value takes exposed sample weight into account, yielding

$$\text{SAR} = \frac{1}{2} \int_V \frac{\sigma(x) |E(x)|^2}{\rho(x)} \, dx \quad (2.2.51)$$

where $\rho$ is the sample density.

The absorbed power can be estimated using the unloaded and loaded Q factors [36]:

$$P_{\text{abs}} = P_{\text{in}} \cdot \left(1 - \frac{Q_l}{Q_u}\right) \quad (2.2.52)$$

Especially at higher fields it is of the utmost importance to accurately calculate the possible SAR values, or potential SAR hotspots to prevent harming the patient.
2.2.5.1 Safety Regulations

In order to avoid local tissue heating and thermo-regulatory affliction, the International Electrotechnical Commission (IEC) has published guidelines [37] for the safe operation of MRI equipment. Limits for the SAR are stated for the whole body, the head, and in any 1-g and 10-g tissue volume, due to different levels of circulation. The IEC defines three different operating modes, which are stated in Tab. 2.5.

<table>
<thead>
<tr>
<th>Operation Mode</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal mode</td>
<td>No stress for the patient</td>
</tr>
<tr>
<td>1st level controlled</td>
<td>&quot;... can cause physiological stress to patients which needs to be controlled by medical supervision&quot;</td>
</tr>
<tr>
<td>2nd level controlled</td>
<td>&quot;potentially significant risk for patients, for which explicit ethical approval is required&quot;</td>
</tr>
</tbody>
</table>

**Table 2.5:** The three different operation modes defined by the IEC.

All transmit coils are separated into two groups of coils, namely volume coils and local coils. For the exact description of those groups refer to [37]. The applicable limits can be seen in Tab. 2.6.

<table>
<thead>
<tr>
<th>Coil Type</th>
<th>Volume</th>
<th>Local</th>
<th>SAR Type</th>
<th>Body Region</th>
<th>Operating Mode</th>
<th>Whole Body SAR</th>
<th>Partial Body SAR</th>
<th>Head SAR</th>
<th>Local SAR (10 g)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Normal</td>
<td>(W/kg)</td>
<td>(W/kg)</td>
<td>(W/kg)</td>
<td>(W/kg)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1st level controlled</td>
<td>2-10a</td>
<td>4-10a</td>
<td>3.2</td>
<td>10b</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2nd level controlled</td>
<td>4</td>
<td>&gt;4</td>
<td>&gt;3.2</td>
<td>&gt;20b</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Short Duration MR examination</td>
<td>The SAR limits over any 10 s period shall not exceed 2× the stated values</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table 2.6:** The SAR limits as stated by the IEC. The averaging time for the above stated limits is 6 min. The exposed mass is defined as the volume where 95% of the RF power is deposited. The local SAR is averaged over a mass of 10 g.

The superscripts in Tab. 2.6 denote:

- **a** The limit scales dynamically with the ratio exposed patient mass/patient mass:
  
  Normal operating Mode:  \[ \text{Partial body SAR} = 10 \text{ W/kg} - \frac{8 \text{ W/kg} \cdot \text{exposed mass}}{\text{total mass}} \] \hspace{1cm} (2.2.53)

  1st level controlled:  \[ \text{Partial body SAR} = 10 \text{ W/kg} - \frac{6 \text{ W/kg} \cdot \text{exposed mass}}{\text{total mass}} \] \hspace{1cm} (2.2.54)

- **b** In cases where the orbit is in the field of a small local RF transmit coil, care should be taken to ensure that the temperature rise is limited to 1 °C.
2. Theoretical Background

2.2.6 RF Probe Designs

Ever since NMR was discovered to be applicable for biomedical investigations, numerous RF coil designs were introduced and published. Some of them were specifically designed for certain anatomical regions, some to cover a wide range of possible application areas. As already seen in the safety regulations, there are two main types of RF coil designs: volume and surface coils.

2.2.6.1 Volume Coils

Volume coils are commonly used to achieve a homogeneous $B_1$ field in a large volume of interest (VOI). Physically, the sample is inserted into the volume coil, therefore demanding differently sized coils for different sized samples. The easiest realization of a volume coil is a simple loop wrapped around a sample, a little more elaborate are the solenoid types (Fig. 2.24a, [5]), which provide high sensitivity but at the same time requires the coil to be orthogonally oriented to the $B_0$ field direction, and saddle coil designs (Fig. 2.24b, [38]). The most prominent example of a volume coil is the birdcage resonator (Fig. 2.24c), firstly introduced in 1985 by Hayes et al. [39].

A birdcage coil is of cylindrical shape with rings of conducting wire or tape at the top and bottom (end rings). The rings are connected by evenly distributed straight rungs also called legs. The coil is tuned by capacitors. Depending on the position of these capacitors, there are three types of birdcage resonators, the low pass (capacitors on the legs), the high pass (capacitors between legs in the end rings), and the band pass birdcage as a combination of the two. Typical birdcages are constructed with a number of 12-24 legs. The ratio of the number of legs to the coil diameter has an influence on the achievable RF field homogeneity [40].

![Figure 2.24: Three volume coil designs](a) Solenoid (b) Saddle (c) Birdcage)

2.2.6.2 Surface Coils

A surface coil is a probe that is placed directly on the surface of the sample under investigation. In 1980, Ackerman et al. [41] showed that the use of simple surface loops for
biomedical investigation of $^{31}\text{P}$ metabolites in animals, achieves much higher SNR than a volume coil could. This is due to the size of the surface coils and the consequentially smaller field of view, which results in less noise contribution from coil and sample.

The disadvantage of surface coils is that the $B_1$ field distribution is intrinsically inhomogeneous. Close to the coil wires the field intensity is high, rapidly falling off when moving further into the sample.

The simplest representation of a surface coil is a loop or rectangle made of copper wire with capacitors distributed along its circumference. The inductance is determined by the coil geometry and the capacitors can be used to tune the coil to the needed Larmor frequency. Distributing several capacitors along the loop, yields a more even current distribution, and as a result a more uniform $B_1$ field. Additionally, these discretely distributed capacitors help to minimize conservative $E$-fields, caused by electrical potential on conductors. Those conservative $E$-fields give rise to sample loss called dielectric loss [29]. Together with the magnetically induced electrical field, which is produced by the time-varying magnetic field, they form the total $E$ field. Sample loss resulting from the magnetically induced $E$ field are called inductive loss. As a rule of thumb, the distance between two subsequent capacitors should not exceed $\lambda/20$ of the respective wavelength.

### 2.2.6.3 RF coil arrays

The application of surface coils has shown to provide high SNR over a limited field of view (FOV). In order to cover a larger FOV while maintaining the high SNR, coil arrays were introduced [42]. The signal received by each individual coil element is combined to obtain a total signal from the FOV. In the case of a transmit array, in order to achieve a more homogenous $B_1$ pattern, the phase of each channel can be adjusted to obtain a certain optimal pattern (static $B_1$ shimming).

Additional advantages of array coils are the possibility to employ parallel imaging [43] and/or transmission [44] techniques. Parallel imaging techniques can be used to speed up the acquisition at the cost of increased image noise. Parallel transmission (pTx) was introduced in 2003 by Katscher et al. [45], and can be used to excite an arbitrarily chosen pattern yielding a more homogeneous excitation field. To achieve this the driving voltages of each channel are variable in amplitude and phase (dynamic $B_1$ shimming), which gives rise to complicated SAR patterns that need to be accurately simulated before scanning.

The individual coil elements of an array are usually placed in close vicinity, yielding mutual coupling [46]. When two coils are mutually coupled, the current in one coil induces a voltage in the other (see Fig. 2.25).

This coupling can be represented as a mutual impedance $Z_{21}$ defined as the ratio of the
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The mutual coupling of two coils described by the coupling coefficient $M_{12}$. The current in coil 1 ($I_1$) induces a voltage in coil 2 leading to current flow $I_2$.

**Figure 2.25:** The mutual coupling of two coils described by the coupling coefficient $M_{12}$. The current in coil 1 ($I_1$) induces a voltage in coil 2 leading to current flow $I_2$.

induced voltage in coil element 2 to the current flowing in coil element 1:

$$Z_{21} = \frac{V_2}{I_1} = R_{21} + iX_{21} \quad (2.2.55)$$

Like the self-impedance described in section 2.2.3, the mutual impedance consists of a resistive ($R_{21}$) and reactive ($X_{21}$) part. The reactive part can either be inductive or capacitive and can cause splitting of the initially single resonance frequency to two resonances corresponding to in-phase and opposed-phase currents in the two coils; this phenomenon is called "peak splitting". This reduces the probe’s sensitivity at the Lamor frequency. The resistive part induces noise correlation between elements, reducing the total SNR. It is, therefore, beneficial to eliminate or at least reduce the mutual coupling.

How strongly two coil elements influence each other is described using the coupling coefficient $k$ defined as

$$M_{12} = k\sqrt{L_1L_2} \quad (2.2.56)$$

The voltage at the output of coil 1 (Fig. 2.25) can be described ba [47]:

$$V_{out} = V_{signal} + \left( R_1 + i\left( \frac{\omega L_1 - \frac{1}{\omega C_1}}{N_{coil}} \right) I_1 + i\omega M_{12}I_2 \right) \quad (2.2.57)$$

The noise associated with coil 1, i.e. $N_{coil}$, can be minimized by tuning and matching coil 1 to the Larmor frequency, thereby equating $\omega L_1$ to $1/\omega C_1$ so that only the intrinsic resistance $R_1$ remains. The noise contributed due to coupling of neighboring coils is represented in the term $N_{coupling}$. It is the goal of decoupling to minimize term $N_{coupling}$.

There exist a variety of methods for reducing mutual coupling effects, three of the most common include overlapping coils [42], shared L/C elements [48], and transformers [49]. In case of a receive only coil array, mutually coupled elements can be decoupled using preamplifier decoupling [42, 47].

**Overlap Decoupling**

Overlap decoupling was first proposed by Roemer et al. in his seminal paper "The NMR phased array" [42]. The idea is that two adjacent coils should be overlapped, so that they
share a common area. The magnetic flux in this shared area can then cancel the magnetic flux through the non-overlapped area, reducing the inductive coupling. An estimation of the overlap area for circular and square loops is given in Fig. 2.26

\[ \text{Overlap distance: } 0.75 \cdot d \quad \text{and} \quad 0.9 \cdot l \]

**Figure 2.26:** The overlap distance necessary to reduce mutual coupling effects for circular loops is roughly \(0.75 \cdot d\) and \(0.9 \cdot l\) for square loops [42].

Due to very subtle geometry differences the exact overlap has to be determined empirically on the bench.

One obvious disadvantage of this widely used decoupling method is the applicability only to adjacent coil elements, next nearest neighbors can not be decoupled using overlap. Also overlap decoupling can only reduce magnetic coupling effects but not the electric coupling due to the electric fields.

**Inductive and Capacitive Decoupling Networks**

When the mutual coupling effect is regarded as a mutual impedance \(Z_{ij}\) between coil elements, inductive or capacitive decoupling networks can be used to reduce this mutual impedance, by sharing either a capacitor or inductor to minimize \(Z_{ij}\). In Fig. 2.27 three such decoupling networks are represented in a simplified matter.

**Figure 2.27:** Three Decoupling methods employing inductive or capacitive networks.

**Preamplifier Decoupling**

The previously mentioned decoupling methods conceptually attempt to minimize the mutual coupling between two coils \(M_{12}\) in order to minimize term 2 of equation (2.2.57). Using the preamplifier to decouple two coils corresponds to \(I_2 = 0\), and therefore minimizes the noise due to mutual coupling. Coil 2 in Fig. 2.28 is equipped with a low noise preamplifier. \(L_2\) and \(C_2\) are used to match the coil impedance to 50 \(\Omega\) when looked at from the preamp itself. Additionally, \(L_2\) and \(C_2\) constitute a parallel resonant circuit when
the preamp input impedance is small (\( r_{\text{amp}} \) around 0 - 2 \( \Omega \)). In this case the impedance seen from the coil is very high. A high impedance circuit acts like a open circuit and thereby prevents any current flow, i.e. \( I_2 = 0 \).

Figure 2.28: Preamp decoupler prevents current flow (\( I_2 \)) in coil 2, therefore minimizing the noise contribution due to coupling.

Since the preamplifiers are highly sensitive to high voltages, this decoupling technique is only usable for receive only coil arrays.

### 2.2.6.4 Noise Correlation

Even if the mutual inductance of array coil elements is zero, there still exist a mutual resistance between them, leading to correlation of noise. This noise correlation can result in a degradation of the combined image/spectra SNR [42]. In order to achieve high SNR in the composite data, the noise correlation matrix can be calculated and later used offline for reconstruction of the combined data [42, 50].

In general, for an \( M \) element array, the signal and noise measured in a pixel located at \( x \) by the coil element \( a \) can be described in complex notation by

\[
S_a(x) = s_a(x)e^{i\phi_a(x)} \quad N_a(x) = n_a e^{i\phi_a} \tag{2.2.58}
\]

It is assumed that \( n_a \) and \( \phi_a \) are fully independent random variables [51]. All the other variables are dependent on the voxel position \( x \). Now, the noises of two coil elements \( a \) and \( b \) are random but not uncorrelated variables. Consider a conductive sample in the vicinity to coil element \( a \) and \( b \). Random charge movements in the sample induce noise voltages with the same phase in both elements due to a fluctuating magnetic dipole moment. These two noises are correlated to some extent. The average noise power \( N_P \) can be written as [51]

\[
N_P = \langle (N_a + N_b)(N_a + N_b)^* \rangle = \langle n_a^2 \rangle + \langle n_b^2 \rangle + 2\langle n_a n_b \cos(\phi_a - \phi_b) \rangle \tag{2.2.59}
\]

the angular brackets \( \langle \rangle \) denote an ensemble average. The correlation term accounts for any correlation between the noises. The so called correlation coefficient \( r_{ab} \) can be defined as

\[
r_{ab} = \frac{\langle n_a n_b \cos(\phi_a - \phi_b) \rangle}{\sqrt{\langle n_a^2 \rangle \langle n_b^2 \rangle}} \tag{2.2.60}
\]
2.2 Radio Frequency Coil Design

![Diagram of coil combination](image)

**Figure 2.29:** Schematic signal combination of data received with an array coil.

The $r_{ab}$, for $a, b = 1, ..., M$ are the matrix coefficients of the noise correlation matrix $R_{nc}$. The noise correlation matrix can be used to maximize SNR of the final image /spectra acquired by an RF coil array [51, 52, 53].

**Signal Combination**

When an array coil is used for reception, in most cases the individual signals have to be combined to yield one composite signal/image. To achieve better results in terms of SNR, the individual signals of coil elements $i$ might be weighted by some complex value $w_i$ before they are summed up (see Fig. 2.29).

The knowledge of the noise correlation can be used to choose the weighting factors accordingly [42, 51, 31]. I refer the reader to Rodgers and Robson [53] for an elaborate review on current state-of-the-art coil combination methods.

**2.2.7 Connecting the Probe to the Scanner**

Once the RF probe is built and resonant at the specific Larmor frequency, it has to be connected to the scanner hardware. This connection includes transmit receive switches, in case of a transmit-receive coil, preamplifiers for signal amplification, and possibly power splitters in case of transmit arrays. The necessity of matching the impedance of the coil to the scanner hardware’s impedance, usually 50 $\Omega$ in MR systems, was already described in section 2.2.3.2.
Preamplifier

Once the signal is detected with the available SNR it is necessary to amplify the intrinsically small signal without further degradation. The voltage induced in the coil is of the order of a few mV [47]. This small signal is amplified to a higher voltage by an amplifier with a gain of (typically) 30 dB. It is placed in the receive path to do this. The preamplifier itself adds noise to the signal, which is indicated by its noise figure (NF) on a dB scale [54]

\[
NF = 20 \log_{10} \left( \frac{SNR_{in}}{SNR_{out}} \right)
\]  

(2.2.61)

The impedance of the coil should be matched to a certain preamplifier input impedance \(Z_N\) for an optimal system noise figure. This so-called noise matching can be achieved by employing the techniques of the previously described impedance matching, i.e. transforming the coil impedance to \(Z_N\). When noise matching was successful it ensures optimal SNR performance of the receive chain. For a lot of commercial preamplifiers this optimal noise impedance value is adjusted to 50 \(\Omega\). An ideal preamplifier has a noise figure of 0, realistic devices have noise figures around 0.3-0.5 dB [47]. Since any passive element within the RF coil generates noise, e.g. cables, the preamplifiers should be placed as close to the RF coil as possible, in order to minimize additional noise contribution.

Transmit/Receive Switch

In case of an RF coil that is used for transmission and reception, there is the need for a switch (T/R switch) to change between the correct signal paths. Additionally, this switch is used to prevent any harm to the sensitive preamplifiers due to the high voltages occurring in the transmit path, which can be up to 8 orders of magnitude higher than the receive signal.

Common T/R switch designs are based on quarter wavelength transmission lines and crossed diodes [55] or PIN diodes [5, 33]. Fig. 2.30a depicts the schematic of \(\lambda/4\), PIN diodes switch. In transmit mode, the PIN diodes \((D_1, D_2)\) are closed due to the direct current supplied by the DC supplier, usually about 10-100 mA. When \(D_1\) is closed, the transmit signal can pass to the coil, while the closed \(D_2\) PIN diode shortens the preamplifier input to ground. The \(\lambda/4\) transmission line (TL) is used as an impedance transformer, converting the low impedance of the mentioned short circuit to a very high impedance at the end of the TL. The high impedance protects the preamplifier from the powerful transmit signal. In receive mode, both PIN diodes are open, letting the receive signal pass directly to the preamp.
Power Splitter

Typical MR system are equipped with only one transmit channel. In order to operate an array coil, this single transmit channel has to be split into several individual channels. A simple method to achieve a low loss splitting is the Wilkinson power divider (WPD) [56]. The WPD again utilizes quarter wavelength transmission lines. It can be used to either split the transmit power into equal or unequal parts. A possible configuration for a three way WPD is shown in Fig. 2.30b. The three way splitter consists of three λ/4 TLs with a characteristic impedance of $\sqrt{3}Z_0$, where $Z_0$ is the characteristic impedance of the system, and three resistors with a resistance of 3-times $Z_0$. This yields an equal three way splitter, matched to 50 $\Omega$.

2.2.7.1 Baluns and Cable Traps

To relate the RF coil to the scanner as described above, coaxial cables are used. A coaxial cable itself is an unbalanced structure, i.e. the current on one signal path works against ground, resulting in nonzero net current. Connecting the shield of a coax cable to an ideally balanced coil, as is done for impedance matching, results in an unbalanced circuit, which gives rise to common mode currents. This common mode degrades the performance of the RF coil in various ways, e.g. inducing additional loss sources, modifying tuning and matching, additional noise. For in vivo studies common mode currents on the shield of the cables are a safety risk, and may cause severe burns [33].

To prevent common mode currents, baluns (balanced to unbalanced transformers) or cable traps can be employed [5, 33]. Different balun designs exist, some of them can also be used as impedance transformers replacing the standard matching network. Another possibility to block the common mode currents on the cable braids are the so-called cable traps. The simplest cable traps are ferrite chokes, which, unfortunately, are not MR compatible. The
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half-wave loop balun shown in Fig. 2.31a is a 4:1 impedance transformer, meaning there is 4 times the characteristic impedance on the balanced side. The quarter-wave balun in Fig. 2.31b is a 1:1 transformer often called bazooka balun. Fig. 2.31c and 2.31d show two designs for current blocking circuits. The trap depicted in Fig. 2.31d has the advantage that it is not soldered or connected to the coaxial cable itself, and can be placed anywhere [57].

![Baluns and Cable Traps](image)

**Figure 2.31:** Baluns and cable traps for preventing common mode currents.

**Summary**

This chapter has provided some theoretical and practical background for RF coil engineering. The principle of transmitting and receiving signals has been reviewed, as well as basic electronics for RF circuits necessary to understand how tuning, matching, and decoupling is achieved. Also the regulatory limits for the specific absorption rate, that have to be abode at all costs, are stated. The technical instruments needed to connect an RF coil with the scanner hardware, e.g. power splitters, T/R switches, preamplifiers, cable traps, etc., are described. The information in this chapter should hopefully suffice to understand the electrotechnical considerations necessary for RF coil development.
2.3 Numerical Simulation

The electromagnetic fields produced by the RF coil in NMR are naturally interacting with biological tissues. This results in a variety of effects influencing image quality and even patient safety. With the current trend towards higher static magnetic field strength to improve the signal-to-noise ratio, the calculation of these effects have gained in importance.

In the early years of RF coil simulation, the main approach consisted of applying Kirchhoff’s current and voltage laws for an RF circuit, and assuming a spatially uniform current distribution in the coil conductors. The electromagnetic fields can then be reliably derived from the uniform current distribution on the conductors with Biot-Savart’s law \[39, 58\] and eq. (2.2.18). Since interaction of the EM fields with biological tissue is relatively weak at low frequencies, this approach is valid even in presence of a load. This quasi-static approximation holds as long as the wavelength is larger than the sample space, e.g. at 1.5 T the wavelength of the proton Larmor frequency (\(\approx 64\) MHz) in muscle tissue is approximately 55 cm, which in most cases is far larger than the sample. The tissue wavelength can be calculated with the knowledge of its relative permittivity \(\varepsilon_r\), its relative permeability \(\mu_r\), and the free space wavelength \(\lambda_0\),

\[
\lambda_{\text{tissue}} = \frac{1}{\sqrt{\varepsilon_r\mu_r}} \cdot \lambda_0 \quad (2.3.1)
\]

The relative permittivity is a frequency dependent function and is different for various tissue types, such as muscle and brain (see Fig. 2.32a). In this work the ITIS Foundation tissue properties database was used for all biological tissue values. The dielectric parameters \((\varepsilon_r, \sigma)\) are based on the measurements published by Gabriel [59]. Due to the decreasing behavior of \(\varepsilon_r\) and the relation to \(\lambda_{\text{tissue}}\), the tissue wavelength also decreases with increasing frequency (see Fig. 2.32b). For example in gray matter, \(\lambda_{\text{GM}}\) is approximately 47 cm, 27 cm, and 13 cm at 1.5 T, 3 T, and 7 T, respectively.

One consequence of the shortened wavelength is that quasi static approximations deviate from measured data. Also with increasing field strength, and hence, decreasing wavelength, the \(B_1^+\) homogeneity starts to deteriorate, and tissue becomes more prone to localized heating as a result of electromagnetic absorption. Designing RF coils for high fields therefore demands a more complex treatment, such as full wave three dimensional (3D) electromagnetic (EM) simulation [60], employing methods like the finite difference time domain method (FDTD) [3].

2.3.1 Electromagnetic Basics

The basis for RF coil modeling are the well known time dependent Maxwell’s equations in matter, which are a set of four coupled partial differential equations and three material
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![Graphs showing relative permittivity and tissue wavelength as functions of frequency.]

(a) Relative permittivity as a function of frequency.

(b) Tissue wavelength as a function of frequency.

Figure 2.32: Relative permittivity (left) and wavelength (right) for white and gray matter, muscle and bone tissue as a function of frequency. The three vertical gray lines are positioned at 64 MHz, 128 MHz, and 298 MHz corresponding to the \(^1\)H Larmor frequency at 1.5 T, 3 T, and 7 T, respectively.

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laws, describing the interaction between electric (\(E\)) and magnetic (\(H\)) fields and the influence of total currents and charges. The Maxwell equations are formed by 4 laws,

\[
\nabla \cdot D = \rho_c \quad \text{(Gauss’s law)} \quad (2.3.2)
\]

\[
\nabla \cdot B = 0 \quad \text{(Gauss’s law for magnetism)} \quad (2.3.3)
\]

\[
\nabla \times E = \frac{\partial B}{\partial t} \quad \text{(Faraday’s law)} \quad (2.3.4)
\]

\[
\nabla \times H = J + \frac{\partial D}{\partial t} \quad \text{(Ampere’s law)} \quad (2.3.5)
\]

together with the material laws.

\[
B = \mu_0 H \quad J = \sigma E \quad D = \varepsilon_0 E \quad (2.3.6)
\]

In general, except for some special cases, analytical solutions of those equations are not known. However, numerical methods in electromagnetism have been established to yield a satisfactory approximation [61]. They either use the integral form of equations (2.3.2) - (2.3.5), e.g. the method of moments (MoM), or the presented partial differential form, e.g. finite difference time domain method (FDTD) or finite element method (FEM).

In all three methods a discretized model of the RF coil and the sample is used to derive the electromagnetic field produced by the RF coil. Among those methods, the FDTD approach is probably the most commonly used, due to its relatively low hardware requirements and ability to model complex multi-material structures, without an impact on computation time. The time dependent Maxwell’s equations are discretized in space and...
numerically solved using central difference approximations to the space and time partial derivatives.

2.3.2 Finite Difference Time Domain Method

All EM simulations in this work employ the FDTD method as described in the following sections. The method was firstly introduced in 1966 by Kane Yee [3], where he described a numerical technique that enables solving Maxwell’s curl equations directly in the time domain on a space grid, with the use of central difference approximations.

2.3.2.1 Discretization in Space

FDTD uses a three dimensional rectangular coordinate system composed of cubes called Yee cells (Fig. 2.33) to discretize the sample space. The following equations are the expanded versions of Faraday’s (eq. (2.3.4)) and Ampere’s (eq. (2.3.5)) law in their vector components

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right); \quad \frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x \right);
\]

\[
\frac{\partial E_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right); \quad \frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} - \sigma E_y \right),
\]

(2.3.7)

where \( E_x, E_y, E_z \) are the x-, y-, and z-components of the electric field \( \mathbf{E} \); the same applies for the magnetic field \( \mathbf{H} \). These equations form the basis for the described method.

In Yee’s FDTD algorithm [3], the electric and magnetic fields are arranged on the Yee cubes by placing the \( \mathbf{E} \) field components in the middle of the edges, and the \( \mathbf{H} \) field components on the center of the faces (Fig. 2.33). Each cell also stores the respective material properties \( (\rho, \sigma, \varepsilon) \).

2.3.2.2 Central Difference Approximations

The Taylor series expansion of a function \( f(x) \) expanded around \( x_0 \) with an offset of \( h/2 \) is given by:

\[
f \left( x_0 \pm \frac{h}{2} \right) = f(x_0) \pm \frac{h}{2} f'(x_0) + \frac{1}{2!} \left( \frac{h}{2} \right)^2 f''(x_0) \pm \frac{1}{3!} \left( \frac{h}{2} \right)^3 f'''(x_0) + \pm + \pm \ldots \quad (2.3.8)
\]

where \( f'(x), f''(x), \) and \( f'''(x) \) denote the first, second, and third derivative, respectively. This directly yields

\[
\frac{f \left( x_0 + \frac{h}{2} \right) - f \left( x_0 - \frac{h}{2} \right)}{h} = f'(x_0) + \frac{2}{3!} \left( \frac{h}{2} \right)^2 f''(x_0) + \ldots \quad (2.3.9)
\]
2. Theoretical Background

Figure 2.33: Schematic of a Yee cell. The Yee cells store the \( H \) field information on the center of the faces and the respective \( E \) field data on the middle of the edges. Dielectric properties of the tissue is also stored for each cell in the computational domain \( \mathcal{C} \)

Rearranging equation (2.3.9) shows the relationship of the first derivative at position \( x_0 \) to the central difference approximation plus a term that is dominated by \( h^2 \), given \( h < 1 \),

\[
\left. \frac{df(x)}{dx} \right|_{x=x_0} = \frac{f(x_0 + \frac{h}{2}) - f(x_0 - \frac{h}{2})}{h} + O(h^2) \quad (2.3.10)
\]

If the offset \( h \) is sufficiently small then the term \( O(h^2) \) can be neglected and a reasonable approximation of the first derivative is given by the central difference

\[
\left. \frac{df(x)}{dx} \right|_{x=x_0} \approx \frac{f(x_0 + \frac{h}{2}) - f(x_0 - \frac{h}{2})}{h} \quad (2.3.11)
\]

2.3.2.3 Yee’s FDTD algorithm

Notation: A point in the discretized three dimensional sample space will be denoted as

\[
(i, j, k) = (i\Delta x, j\Delta y, k\Delta z) \quad (2.3.12)
\]

where \( \Delta x, \Delta y, \Delta z \) are the spatial steps (the length of the cell edges) in the \( x, y, \) and \( z \) direction, respectively. A function of space and time evaluated at a discrete point \( (i, j, k) \) at time point \( n \) is written as

\[
F^n(i, j, k) = F(i\Delta x, j\Delta y, k\Delta z, n\Delta t) \quad (2.3.13)
\]

where \( \Delta t \) is the applied time step.

With this notation the time and space derivatives of a function \( F \) approximated with finite central differences (eq. (2.3.11)) can be written as follows. In case of the first partial space derivative in the \( x \)-direction is given by

\[
\frac{\partial F}{\partial x}(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = \frac{F^n_{i+\frac{1}{2},j,k} - F^n_{i-\frac{1}{2},j,k}}{\Delta x} \quad (2.3.14)
\]
2.3. Numerical Simulation

Analogous the y and z derivatives are obtained by changing the indexes j and k accordingly. In case of a time derivative at a fixed location \((i, j, k)\) this yields

\[
\frac{\partial F}{\partial t}(i \Delta x, j \Delta y, k \Delta z, n \Delta t) = \frac{F_{i,j,k}^{n+\frac{1}{2}} - F_{i,j,k}^{n-\frac{1}{2}}}{\Delta t}
\]  \((2.3.15)\)

For example, the first time derivative of the magnetic component \(H_x\) of eqn. \((2.3.7)\) discretized using the finite central differences for the time and space derivatives as described in equations \((2.3.14)\) and \((2.3.15)\) yields

\[
\frac{H_{x|i,j,k}^{n+\frac{1}{2}} - H_{x|i,j,k}^{n-\frac{1}{2}}}{\Delta t} = \frac{1}{\mu_{i,j,k}} \left( \frac{E_{y|i,j,k+\frac{1}{2}}^{n} - E_{y|i,j,k-\frac{1}{2}}^{n}}{\Delta z} - \frac{E_{z|i,j+\frac{1}{2},k}^{n} - E_{z|i,j-\frac{1}{2},k}^{n}}{\Delta y} \right)
\]  \((2.3.16)\)

Rearranging this equation and analogously doing the same procedure for the \(H_y\) and \(H_z\) components yields the discretized magnetic part of the curl equations (eq. 2.3.7):

\[
H_{x|i,j,k}^{n+\frac{1}{2}} = H_{x|i,j,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_{i,j,k}} \left( \frac{E_{y|i,j,k+\frac{1}{2}}^{n} - E_{y|i,j,k-\frac{1}{2}}^{n}}{\Delta z} - \frac{E_{z|i,j+\frac{1}{2},k}^{n} - E_{z|i,j-\frac{1}{2},k}^{n}}{\Delta y} \right)
\]  \((2.3.17)\)

\[
H_{y|i,j,k}^{n+\frac{1}{2}} = H_{y|i,j,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_{i,j,k}} \left( \frac{E_{z|i,j,k+\frac{1}{2}}^{n} - E_{z|i,j,k-\frac{1}{2}}^{n}}{\Delta x} - \frac{E_{x|i,j+\frac{1}{2},k}^{n} - E_{x|i,j-\frac{1}{2},k}^{n}}{\Delta z} \right)
\]  \((2.3.18)\)

\[
H_{z|i,j,k}^{n+\frac{1}{2}} = H_{z|i,j,k}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_{i,j,k}} \left( \frac{E_{x|i,j,k+\frac{1}{2}}^{n} - E_{x|i,j,k-\frac{1}{2}}^{n}}{\Delta y} - \frac{E_{y|i,j+\frac{1}{2},k}^{n} - E_{y|i,j-\frac{1}{2},k}^{n}}{\Delta x} \right)
\]  \((2.3.19)\)

When the initial condition is known, e.g. all field values are 0 at time point \(t = 0\), then the right hand sides of the equations are known and the updated field value can directly be calculated.

Analogous to equation \((2.3.16)\) the first partial time derivative of the electric field component \(E_x\) at a spatial position \((i, j, k)\) is given by:

\[
\frac{E_{x|i,j,k}^{n+1} - E_{x|i,j,k}^{n}}{\Delta t} = \frac{1}{\varepsilon_{i,j,k}} \left( \frac{H_{x|i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_{x|i,j,k-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y} - \frac{H_{y|i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_{y|i,j,k-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z} - \sigma_{i,j,k} E_{x|i,j,k}^{n+\frac{1}{2}} \right)
\]  \((2.3.20)\)

The magnetic field values are evaluated at time step \(n+1/2\) and are obtained by equations \((2.3.18)\) and \((2.3.19)\). The electrical field term on the right hand side is also evaluated at \(n + 1/2\), which has to be approximated:

\[
E_{x|i,j,k}^{n+\frac{1}{2}} = \frac{E_{x|i,j,k}^{n+1} + E_{x|i,j,k}^{n}}{2}
\]  \((2.3.21)\)

Again rearranging equation \((2.3.20)\) and substituting equation \((2.3.21)\) yields the updated
with the material property coefficients

\[
\alpha_{i,j,k} = \frac{1 - \frac{\sigma_{i,j,k}\Delta t}{2\varepsilon_{i,j,k}}}{1 + \frac{\sigma_{i,j,k}\Delta t}{2\varepsilon_{i,j,k}}} \quad \beta_{i,j,k} = \frac{\Delta t}{1 + \frac{\sigma_{i,j,k}\Delta t}{2\varepsilon_{i,j,k}}}
\]

Since the magnetic field components \(H_x\), \(H_y\), and \(H_z\) were calculated in the previous step (eq. (2.3.17) - (2.3.19)), the right hand side of the set of equations above is known, and the electric field components can be explicitly calculated.

\[E^{n+1}_x[i,j,k] = \alpha_{i,j,k}E^n_x[i,j,k] + \beta_{i,j,k} \left( \frac{H^{n+\frac{1}{2}}_y[i,j,k] - H^n_y[i,j,k+\frac{1}{2}]}{\Delta y} - \frac{H^{n+\frac{1}{2}}_z[i,j,k] - H^n_z[i,j,k-\frac{1}{2}]}{\Delta z} \right) \]

\[E^{n+1}_y[i,j,k] = \alpha_{i,j,k}E^n_y[i,j,k] + \beta_{i,j,k} \left( \frac{H^{n+\frac{1}{2}}_x[i,j,k] - H^n_x[i,j,k-\frac{1}{2}]}{\Delta x} - \frac{H^{n+\frac{1}{2}}_z[i,j,k] - H^n_z[i,j,k-\frac{1}{2}]}{\Delta z} \right) \]

\[E^{n+1}_z[i,j,k] = \alpha_{i,j,k}E^n_z[i,j,k] + \beta_{i,j,k} \left( \frac{H^{n+\frac{1}{2}}_x[i,j,k] - H^n_x[i,j,k+\frac{1}{2}]}{\Delta x} - \frac{H^{n+\frac{1}{2}}_y[i,j,k] - H^n_y[i,j,k+\frac{1}{2}]}{\Delta y} \right) \]  

(2.3.22)  
(2.3.23)  
(2.3.24)

Figure 2.34: Schematic of Yee’s FDTD algorithm. In the initial state all fields are set to 0. After excitation some edges are assigned a value different from 0 and the iterative calculation of the \(H\) and \(E\) fields begin.
Figure 2.34 shows a schematic of the algorithm. The initial condition at \( t = 0 \) is that all fields are set to 0. Only after feeding the system some kind of waveform, some cell edges are assigned an electrical field value not equal to 0.

The iterative process (Steps 3-5) in Fig. 2.34 for a one dimensional problem is illustrated in Fig. 2.35. The electrical field data in the computational domain calculated from previously derived magnetic field data, is stored in memory for a specific time point. This information is then used to calculate all the \( \mathbf{H} \) components in the entire computational space and stored again in memory. The circle begins again with computing all the \( \mathbf{E} \) components based on the newly derived \( \mathbf{H} \) field. This iteration continues until the predefined end (\( t_{\text{end}} \), Step 5) is reached.

\[
\begin{align*}
E & \quad t = 0 \\
E & \quad t = \Delta t \\
E & \quad t = \frac{3}{2}\Delta t \\
E & \quad t = \frac{1}{2}\Delta t \\
E & \quad t = 2\Delta t
\end{align*}
\]

\[
\begin{align*}
x = 0 & \quad x = \frac{1}{2}\Delta x \\
x = \Delta x & \quad x = \frac{3}{2}\Delta x \\
x = 2\Delta x &
\end{align*}
\]

Figure 2.35: Yee’s FDTD algorithm for a one dimensional problem. The use of central differences for the space derivatives.

### 2.3.2.4 Boundary condition

Since it is not possible to numerically compute infinite spaces, proper boundary conditions have to be introduced in numerical simulations in order to truncate the computational domain \( C \). Especially with wave equations, using periodic or hard wall boundary conditions, such as Dirichlet or Neumann conditions, would lead to artifacts from boundary reflections (see Fig. 2.36a). Therefore, the use of absorbing boundary conditions could be defined at the outer lattice to simulate an infinite extension of \( C \). Some promising candidates to achieve this condition have been proposed [60, chapter 6]. Those boundary materials have the function of absorbing the radiating waves, without reflecting them back into the region of interest, while preserving a feasible grid resolution (Fig. 2.36b). In 1994, Berenger [62] introduced his version of the absorbing material and named it perfectly matched layers (PML). The main advantage of these PMLs is that they can be used
2. Theoretical Background

2.3.2.5 Grid Size

The determination of the optimal discretization grid size is an important step when setting up the FDTD simulation. The cell size directly determines two crucial parameters of the simulation, namely the time step size and the upper frequency limit [60, 63]. The grid size should be chosen to be small enough to represent the modeled structure in a realistic way. Figure 2.37a - 2.37b shows two different grid sizes, i.e. 10 mm and 2 mm, discretizing a sphere with a radius of 10 cm. The finer the grid, the more the meshed structure approaches shape of the original sphere.

But one has to keep in mind that the grid size strongly influences the required memory as well as overall simulation time. Therefore, a reasonable cell size has to be determined for an accurate simulation. As a rule of thumb, the maximum cell size should not exceed $1/10^{th}$ of the wavelength of interest [63], e.g. in case of proton imaging at 7 T the wavelength in brain tissue is $\approx 13$ cm, hence, the cell size should not exceed 1.3 cm.

In reality the cell size is often dictated by small structures that are necessary to be resolved in the simulation mesh. In Figure 2.37c - 2.37d a cube with dimensions of $10 \times 10 \times 10$ cm$^3$ has a cavity with a width of 5 mm. Choosing a minimal grid size of 5.1 mm (Fig. 2.37c) will not lead to a mesh resolving the cavity, instead using a finer minimum cell size of 4.9 mm (Fig. 2.37d), the cavity can be perfectly resolved in the mesh.
2.3. Numerical Simulation

![Figure 2.37: Example of three FDTD grid sizes for a sphere with \( r = 10 \) cm, and a cube with an edge length of 10 cm.](a) 10 mm  (b) 2 mm  (c) 5.1 mm  (d) 4.9 mm]

2.3.2.6 Numerical Stability

To ensure numerical stability the time increment \( \Delta t \) has to be bound with respect to the spatial increment \( (\Delta x, \Delta y, \Delta z) \). The stability condition for 3D FDTD problems is given by

\[
\Delta t \leq \frac{1}{c \cdot \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}
\]

(2.3.26)

where \( c \) is the speed of light. Assuming a three dimensional cubic-cell space lattice with \( \Delta x = \Delta y = \Delta z = \Delta \), numerical stability is ensured for

\[
\Delta t \leq \frac{\Delta}{c\sqrt{3}}
\]

(2.3.27)

For the conceptual proof the interested reader is referred to literature [60, chapter 4].

2.3.3 Circuit Co-Simulation

As RF coils generally require tuning, matching, and, depending on the number of coils, decoupling, based on lumped circuit components such as capacitors and inductors, a circuit co-simulation approach can be employed in order to avoid numerous time consuming repetitions of the 3D simulations. This linkage has been used for several years in RF antenna optimization where the main focus relies on 2D far field data. For MRI coil design the technique is based on the fact that for linear RF networks and a specific frequency \( \omega \), 3D EM fields are precisely equal in the two following scenarios [64]:

1. 3D EM field data is obtained from 3D EM simulation incorporating the RF networks needed for tuning, matching, and decoupling

2. 3D EM field data is obtained as a weighted superposition of prototype 3D EM fields from a multi-port 3D EMS together with RF circuit co simulation.
For an RF coil simulation, implementing scenario 2, each lumped element \((j = 1, ..., N)\) used for tuning, matching, and decoupling, as well as the driving feeds, are substituted by driving ports with characteristic impedance of \(Z_0 = 50 \, \Omega\). The 3D EM simulation is then executed with one port activated at a time, while all remaining ports are terminated by a load equal to the characteristic impedance. This results in a full scattering parameter matrix \((S_{N \times N})\), and N electric \((E_i)\) and magnetic \((E_j)\) fields for each activated port. In the co-simulation the S-parameter matrix is used by connecting the corresponding RF networks, consisting of the respective lumped elements, to each port. By changing the values of the lumped elements, the RF coil can be tuned, matched, and decoupled. When the desired state is achieved, the electrical properties of each RF circuit node, i.e. current \((I)\) and voltage \((V)\), are calculated. The electromotive force \((\xi)\) of port \(j\) can then be derived as

\[
\xi_j = I_j(\omega) \cdot Z_0 - V_j(\omega)
\]  

(2.3.28)

Having calculated \(\xi\) for each port, the port power \(P_j(\omega)\) and phase \(\varphi_j(\omega)\) can be written as

\[
P_j(\omega) = \frac{|(\xi_j \cdot \xi_j^*)|}{|2 Z_0| P_j^0}
\]

\[
\varphi_j = \angle(\xi_j) - \varphi_j^0
\]

(2.3.29) (2.3.30)

where the prototype port power and phase is denoted as \(P_j^0\) and \(\varphi_j^0\) and is usually set to 0.01 W and 0°, respectively. The asterisk * denotes the complex conjugate, and \(\angle\) the phase angle. Finally the desired \(E\) and \(H\) field data of the RF coil are given as the superposition of the initially calculated EM field data for each port \((E_j\) and \(H_j)\) weighted by the port power and phase:

\[
H = \sum_{j=1}^{N} H_j \cdot \sqrt{P_j(\omega)} \cdot e^{i\varphi_j(\omega)}
\]

(2.3.31)

\[
E = \sum_{j=1}^{N} E_j \cdot \sqrt{P_j(\omega)} \cdot e^{i\varphi_j(\omega)}
\]

(2.3.32)

This approach enables the calculation of the complex electromagnetic fields produced by the RF coil, with only one run of the time consuming full wave 3D simulation, several rapid RF circuit co simulations and a final post-processing step.

In this thesis, three different commercial software products were used to accomplish the goal of each step. For the full wave 3D electromagnetic simulation a software package called XFdttd by Remcom (State College, PA, USA) was used. There exist many other FDTD simulation packages that achieve the same outcome as XFdttd, such as CST Microwave Studio (CST GmbH, Darmstadt, Germany) or SEMCAD X (Speag, Zürich, Switzerland). The RF circuit co-simulation was done in ADS (Advanced Design System,
2.3. Numerical Simulation

Full wave 3D electromagnetic simulation as depicted in Fig. 2.34
▲ model RF coil and the surrounding
▲ substitute all feeding, matching, and tuning networks by ports with 50 Ω impedance

RF circuit co-simulation as described in section 2.3.3
▲ tune, match, and decouple the structure
▲ calculate the EMF and therefore
★ port power $P^\text{port}_j$ and
★ port phase $\phi^\text{port}_j$

Postprocessing
▲ calculate $H$ and $E$ according to equations (2.3.31) and (2.3.32)
▲ evaluate SAR, eq. (2.3.33)

$S$-parameter matrix

Prototype EM fields for each port \{\(H_j, E_j\)\}_{j=1,...,N}

* XFdtd
* ADS
* Matlab

Figure 2.38: 3D EM simulation workflow. The overall simulation process consists of three parts, namely the full wave 3D simulation (blue block) employing the finite difference time domain method using XFdtd, followed by an RF circuit co simulation (violet block) with the software ADS, concluded by the Postprocessing (green block) step in Matlab.

Agilent, Santa Clara, CA, USA), which offers the useful possibility of automated optimization of tuning, matching, and decoupling conditions. As input it takes the $S$-parameter matrix of the simulated 3D system. The final step is the calculation of the magnetic and electric field of the modeled system. For that purpose Matlab (MathWorks Inc., Natick, MA, USA) was used. The simulation workflow employed in this thesis is depicted in Fig. 2.38.

2.3.4 SAR evaluation

For a fast and accurate evaluation of SAR, local power correlation matrices \([65, 66]\) can be employed, yielding accurately averaged volumes of a specified limit, i.e. 10 g. The specific absorption rate, as introduced in eq. (2.2.51), for an $N$ element transmit coil array at a spatial position $x$ averaged over a volume $V$ can be calculated as \([66]\):

$$\text{SAR}(x, t_i) = \frac{1}{V} \int_V \frac{\sigma(x)}{2\rho(x)} \left\| \sum_{c=1}^{N} E_c(x, t_i) \right\|_2^2 \ dV \quad (2.3.33)$$
2. Theoretical Background

where \( t_i \) denotes a TX sample period, and \( E_c \) is the electric field generated by TX channel \( c \). \( E_c \) can also be written in the following form

\[
E_c(x, t_i) = \bar{E}_c(x) \cdot \alpha_c(t_i)
\]  

(2.3.34)

where \( \bar{E}_c(x) \) is the electric field produced by coil channel \( c \) when driven with unit current, \( \alpha_c(t_i) \) is the complex scaling factor representing the waveform sample transmitted at time \( t_i \) to channel \( c \). With this notation eq. (2.3.33) may be written as

\[
SAR(x, t_i) = \frac{1}{V} \int_V \frac{\sigma(x)}{2 \rho(x)} \left\| \bar{E}(x) \cdot \alpha(t_i) \right\|_2^2 \, dV
\]  

(2.3.35)

The matrix \( \bar{E}(x) \) denotes the 3 × N matrix containing the x, y, z field components of each channels electric field, and \( \alpha(t_i) \) is the vector containing the RF waveforms feeded into the respective channel:

\[
\bar{E}(x) = \begin{pmatrix}
\bar{E}_{x,1} & \cdots & \bar{E}_{x,N} \\
\bar{E}_{y,1} & \cdots & \bar{E}_{y,N} \\
\bar{E}_{z,1} & \cdots & \bar{E}_{z,N}
\end{pmatrix}
\]  

(2.3.36)

The square in equation (2.3.35) can be naturally split, yielding

\[
SAR(x, t_i) = \alpha^H(t_i) \cdot \frac{1}{V} \int_V \frac{\sigma(x)}{2 \rho(x)} \underbrace{\bar{E}^H(x) \bar{E}(x)}_{Q(x)} \, dV \cdot \alpha(t_i)
\]  

(2.3.37)

\[
= \alpha^H(t_i) \cdot Q(x) \cdot \alpha(t_i)
\]  

(2.3.38)

where the superscript \(^H\) denotes the conjugate transpose.

The resulting \( Q \)-matrix is hermitian, and positive semidefinite [66]. These matrices are calculated for each voxel in the simulation space. Finally for the local 10 g SAR values (or any other), the \( Q \)-matrices are averaged elementwise over 10 g volumes [67]. This yields one matrix for each 10 g subvolume (\( Q_{10g} \)). This averaging process is rather time consuming, but fortunately has to be performed only once, since the excitation specific parameters are stored not in \( Q \) but rather in \( v \). For each possible excitation the 10 g SAR value for every 10 g subvolume is simply calculated by

\[
v^H Q_{10g} v
\]  

(2.3.39)

This is much faster than calculating the \( E \)-field superposition for each excitation vector followed by the 10 g averaging.
2.3.5 Power balance

The theory and implementation of the power balance as described herein for RF coils was published as "Power balance and loss mechanism analysis in RF transmit coil arrays", Kuehne A, Goluch S, Waxmann P et al. in Magnetic Resonance in Medicine, 2014, E-pub [68].

The division of the total coil loss into the different contributing loss mechanisms can be used to assess coil efficiency and simulation accuracy. Various loss contributions are present in a typical RF coil setup. The incident power is either reflected, radiated in the far field or dissipated. Dissipation happens either in the coil itself or the load or any other present conducting material, where the load dissipation is of course the desired mechanism. In the coil, losses occur in the lumped elements for tuning, matching, and decoupling, or in the copper wiring. The loss tree can be seen in Fig. 2.39.

As already introduced in the previous section, the power losses can be described using power correlation matrices. To quantify the contributions of the different loss sources in Fig. 2.39, each source will be assigned a corresponding Q-matrix.

Poynting’s theorem states the conservation of energy for electromagnetic fields. In case of time harmonic fields, the power balance of a system is represented as the real part of the theorem:

\[
-\frac{1}{2} \iiint_V \text{Re}(J^* \cdot E) \, dV = \frac{1}{2} \iiint_V \sigma(x)|E|^2 \, dV + \frac{1}{2} \iint_{\partial V} \text{Re}(E \times H^*) \, ds \quad (2.3.40)
\]

Using the Q-matrix formalism, each power loss term can be calculated as

\[
P = v^H Q v \quad (2.3.41)
\]

where \(Q\) is the hermitian, positive semidefinite power correlation matrix, and \(v\) are the time dependent driving voltages in vector form.

The forward power can be represented as

\[
P_{\text{fwd}} = v^H \left( \frac{1}{2Z_0} I_N \right) v \quad (2.3.42)
\]
where \( \mathbf{v} \) is the driving voltage amplitude vector, \( Z_0 \) is the characteristic impedance (usually 50 \( \Omega \)), and \( \mathbf{I}_N \) is the \( N \times N \) identity matrix.

Due to imperfect matching some of the forward power is reflected. The \textit{reflected power} can be represented using the system’s scattering parameter matrix (\( \mathbf{S} \)) as

\[
P_{\text{ref}} = \mathbf{v}^H \left( \frac{1}{2Z_0} \mathbf{S}^H \mathbf{S} \right) \mathbf{v} \tag{2.3.43}
\]

The input power of eq. (2.3.40) is then the forward power minus the reflected,

\[
P_{\text{in}} = \mathbf{v}^H (\mathbf{Q}_{\text{fwd}} - \mathbf{Q}_{\text{ref}}) \mathbf{v} \tag{2.3.44}
\]

The voltage vector \( \mathbf{v} \) is related to the scaling factors (\( \alpha \)) derived in the RF circuit co-simulation (sec. 2.3.3) by

\[
\mathbf{v} = \alpha \cdot \sqrt{2Z_0} P_0
\]

where \( P_0 \) is the single channel port power.

The \textit{radiated power} can be calculated as

\[
P_{\text{rad}} = \mathbf{v}^H \left( \frac{1}{4} (\mathbf{Q}_{\text{rad}} + \tilde{\mathbf{Q}}_{\text{rad}}^H) \right) \mathbf{v} \tag{2.3.45}
\]

where the elements of the matrix \( \tilde{\mathbf{Q}}_{\text{rad}} \) are defined as

\[
\tilde{q}_{ij} = \kappa \iint_{\partial V} \mathbf{E}_j \times \mathbf{H}_i^* \, ds \tag{2.3.46}
\]

Finally the \textit{dissipated power} is described dividing the power dissipated in material (\( P_{\text{mat}} \)), e.g. sample, copper, etc., and dissipated in the lumped elements (\( P_{\text{imp}} \)), e.g. capacitors, inductors, and resistors. In case of a lumped element, the dissipated power can be derived from the voltage drop and the current through it, yielding

\[
P_{\text{imp}} = \mathbf{v}^H \left( \frac{k}{4} (\mathbf{I}^H \mathbf{V} + \mathbf{V}^H \mathbf{I}) \right) \mathbf{v} \tag{2.3.47}
\]

where \( \mathbf{V} \), and \( \mathbf{I} \) are the voltage and current matrices, respectively, where the \( i^{\text{th}} \) column contains the voltages and currents of all lumped elements with unit excitation of the \( i^{\text{th}} \) coil element.

The power dissipated in material of any kind can be expressed as

\[
P_{\text{mat}} = \mathbf{v}^H \mathbf{Q}_{\text{mat}} \mathbf{v} \tag{2.3.48}
\]

where the elements of \( \mathbf{Q}_{\text{mat}} \) are calculated as

\[
q_{ij} = \frac{k}{2} \iiint_V \sigma |\mathbf{E}_j| \mathbf{E}_i^* dV \tag{2.3.49}
\]
2.3. Numerical Simulation

This leads to the expression of Poynting’s theorem in quadratic form:

\[ Q_{\text{fwd}} = Q_{\text{ref}} + Q_{\text{rad}} + Q_{\text{mat}} + Q_{\text{imp}} \]  \hspace{1cm} (2.3.50)

Neglecting small numerical errors, this equation has to be fulfilled for an accurate simulation.

Summary

This chapter has provided the theoretical background to the 3D EM simulation method employed in this work. Electromagnetic basics in form of the Maxwell equations and its discretized form were presented before outlining the FDTD simulation method for electromagnetic applications. The RF circuit co-simulation technique and its basic assumptions are shown. Techniques to evaluate the SAR distribution and the concept of the power balance for RF coil simulations are presented.
RF Coil Development Workflow

An overview of the workflow described in this chapter can be seen in Fig. 3.1. The four main blocks (Preparatory Considerations, Numerical Implementation, Hardware Implementation, and MR Performance) will be further described in detail in the upcoming sections.

3.1 Preparatory Considerations

Before designing and building an RF coil, certain preparatory considerations are necessary. Since in the end the coil should be used for a specific experiment, the first thing to consider for fitting design choices is the anatomy, which the coil should be covering. The first question in every RF coil development workflow should be

1) What anatomical region will be the most decisive part for the experiment?

Possible answers would be calf muscle, liver, shoulder, etc. From the size and position of the anatomical region, the size of the overall coil can be derived. Note that the necessary penetration depth ($\zeta$) is determined by the position of the body part. As a rule of thumb the optimal penetration depth of a loop coil is roughly its diameter [69].

$$\zeta_{\text{target}} \approx d_{\text{coil}} \quad (3.1.1)$$

At this point of the coil design, also aspects of patient compliance and other geometry-relevant features should be considered. Sometimes it is beneficial to have a flexible coil for differently sized body parts. Sometimes the opposite is wanted, a very robust coil housing to support weight or movement of extremities. So question number two would be

2) What features concerning coil hardware should the design have?
One of the most important aspects of coil design is the choice of coil type. This includes the decision for a volume or surface coil, an array or single element coil, transceive or transmit only/receive only, and in the case of an array, the number of elements. Volume coils yield very homogeneous excitation and reception fields but lack high sensitivity, whereas surface coils exhibit high sensitivity close to the surface but have an inherently inhomogeneous
3.2. Numerical Implementation

explanation field. A method to tackle the inhomogeneity of surface coils is to build arrays of surface coils [42]. This will increase both homogeneity and achievable SNR, but will not yield the same homogeneity as a volume coil. Another valuable feature of RF surface coil arrays is the possibility of employing parallel imaging [43] and/or transmit methods [44], which can decrease scan time or further increase homogeneity. Hence, the last question is,

3) What is/are the most crucial performance measure(s) for the experiment?

With the answers to these questions, a preliminary design choice can be identified. Since these preparatory considerations are highly dependent on the particular setting, i.e. field strength and the nucleus of interest, available hardware setup, the starting design choice can not be exclusively derived from the three questions above.

Either way, before building the coil it is advisable to start with simulating this preliminary chosen coil setup. This will give first insights to coil performance, possible safety issues, and might also be used to compare different designs without having to waste expensive components like capacitors, pre-amplifiers, TR switches, and of course time.

3.2 Numerical Implementation

The theoretical basis for the numerical implementation workflow step was introduced in section 2.3. In this part of the development workflow, we will make use of the numerical simulation workflow depicted in Fig. 2.38.

3.2.1 FDTD simulation

Most commercial 3D FDTD simulation software packages have a built-in possibility to make use of CUDA-enabled GPU calculation, which can be used to accelerate the computations.

The simulation software usually also provides CAD tools to model the RF coil, the load, and the surrounding hardware. The RF coil should be modeled as accurately and realistically as possible, which includes accurately modeled coil geometry, housing and a number of gaps for capacitor placement (Fig. 3.2a). The cables that are used in reality to connect the coil to the scanner are left out in the simulation intentionally, since they should not contribute to the magnetic and electric field produced by the coil.

For faster simulation an RF circuit co-simulation is used (section 3.2.2), therefore each capacitor and feeding network is substituted by a 50 Ω impedance port (green connection in Fig. 3.2). Since FDTD is a time domain method, it enables the use of broadband (multiple frequencies) calculation. This can be useful when the network properties close
to the Larmor frequency are of particular interest, e.g. for the S-parameter simulation, or if there are expected resonances from other structures that might get close to the coil’s resonance frequency. The center frequency of the broadband waveform fed into these ports is the desired resonance frequency. The bandwidth of the pulse can be chosen freely. The simulation yields $E$ and $B$ prototype fields for each port, and a multi-port S-parameter matrix.

For a realistic outcome, a suitable load has to be chosen. Since the load couples both magnetically and electrically to the coil, the magnetic and electric field simulated within the load is highly dependent on the accuracy of the load model. Depending on the complexity of the anatomical region investigated, one can create a load that is geometrically similar to the anatomical region but consists of a smaller number of different tissue types (Fig. 3.2b), or use anatomical models created for this purpose (Fig. 3.2c). In this work, the voxel models are taken from the virtual family set [70]. They exist in various spatial resolutions from 0.5 mm$^3$ to 5 mm$^3$ consisting of 75-84 tissue types. Each tissue type has characteristic electromagnetic properties depending on the frequency that is used for the simulation.

![Figure 3.2: Four element overlapped RF coil array model with (a) no load, (b) plastic former (blue) and tissue phantom load, and (c) a voxel model load from the virtual family [70].](image)

An important part of a FDTD simulation is the choice of the grid size and consequently the mesh. Generally, the choice of the spatial increment is proportional to the respective wavelength in the medium. In order to accurately simulate wave propagation in the discretized sample, the cell size should not exceed $1/10$ of the wavelength [63, 60]. Although, most often the cell size is more likely determined to adequately resolve the geometry details (see sec. 2.3.2.5), which is often very well below $\lambda/10$ [60]. Since the cell size directly
affects the number of cells and therefore the computation time, it is necessary to find a reasonable compromise between accuracy of the simulation and computation time. Collins et al [71] concluded that for human voxel models at 64 MHz (1.5 T) the local and average SAR resulting from a 5 mm isotropic mesh does not significantly differ from the results of a 2 mm isotropic mesh simulation. For higher frequencies, and with the development of high resolution voxel models (up to 0.5 mm [70]), it has been shown that a mesh size of 2-3 mm isotropic still yields sufficiently accurate results [72]. Kozlov et al. [64], however, even used a 1 mm isotropic mesh for his RF circuit co-simulation work.

In most FDTD simulation software packages the grid, and subsequently the mesh, is generated automatically. The maximum target cell size, as well as the minimum acceptable cell size can be defined for each structure. The automated grid generation will distribute the minimum number of cells for the respective structure, while abiding these limits. Additionally for a given structure, one might define certain fixed points. These fixed points have to be positioned on a cell edge or face by the grid generation algorithm. Most often, these fixed points are set for corners or edges of structures or lumped elements, in order to fully account for those geometric details. In some cases it might be desired that the defined limits are applicable to a certain area surrounding the structure. This area extension in terms of cell size regions will be called boundary extension. This option is often used for coil wires and phantom/voxel models, to assure that there are no mesh size changes immediately after the main structure ends, which could potentially lead to errors.

In this work, the grid size limits chosen for the three main simulation space structures, i.e. the RF coil, the sample, and the air filled cells (padding cells) that fill the space around the RF coil/sample to the simulation space boundary, are chosen according to table 3.1. The

<table>
<thead>
<tr>
<th>Structure</th>
<th>Maximum grid size [mm]</th>
<th>Minimum grid size [mm]</th>
<th>Boundary extension [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coil wire</td>
<td>1</td>
<td>0.5</td>
<td>5-10</td>
</tr>
<tr>
<td>Phantom/voxel models</td>
<td>3</td>
<td>1.5</td>
<td>10-15</td>
</tr>
<tr>
<td>Padding</td>
<td>10</td>
<td>5</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 3.1: Maximum and minimum grid size for different model structures.

simulation space boundary consists of 7-10 perfectly matched layers (PML), to prevent any reflections [60]. Although the PML layers are designed to simulate infinite space by absorbing the outward propagating waves without reflecting them, they are not put in close vicinity to the sample, to avoid possible error due to potential interaction between PML and structure. A number of 10-20 padding cells per direction is usually put between structure and boundary.
With these definitions a resulting grid for an example coil with load is depicted in Fig. 3.3

Figure 3.3: The three grid sizes of a simplified FDTD model. A simple loop coil (orange ring) is placed atop of a phantom (green). The cell lines are depicted in gray. The three model structures and the respective cell sizes are: 1) RF coil, cell size: 0.5 mm - 1 mm, boundary extension: 5 mm. 2) Sample, cell size: 1.5 mm - 3 mm, boundary extension: 10 mm. 3) Padding cells, cell size: 10 mm, number of cells per direction: 18. The boundary extension is the distance between the dashed and the full line. The blue area represents the 7-10 PML absorbing layers surrounding the simulation domain.

Since the FDTD method is a time-stepping method, a termination condition has to be defined when the algorithm stops. This can either be a specified number of time steps, or an automated termination once convergence is reached. The 3D electromagnetic simulation calculates the response of the RF coil to an input pulse. The energy fed via the broadband pulse to the coil is distributed across the system, and is dissipated in the lossy coil and sample or radiated into the far field. Therefore it makes sense to terminate once the remaining energy of the system, which is quantified as the algebraic sum of the available power of all active ports, reaches some kind of convergence level [73]. This level of convergence is monitored in a first test run. The test run differs from the final simulation only in defining no termination criterion, so the simulation would run infinitely. The net available power is monitored until it reaches a level of -90 dB. The time step where this condition is met is then manually set as the termination criterion for the final simulation set up. This way it is assured that no early termination error alters the simulation results.

For the RF circuit co-simulation described in the next section only the S-parameter matrix at the frequency of interest of the system is required.
3.2.2 RF circuit co-simulation

The RF circuit co-simulation enables time consuming tuning and matching outside of the FDTD simulation. Kozlov et al. [64] showed the feasibility of that method for the simulation of MR coils. The theory was described in more detail in section 2.3.3.

A straightforward implementation of this procedure in Matlab was recently published [74]. In this work, Agilent ADS was used.

The circuit co-simulation comprises two simulations

1. Scattering parameter (S-parameter) simulation: to tune and match the RF coil
2. Alternating current (AC) simulation: to calculate the scaling factors

For both simulations, the S-parameter matrix from XFDTD is imported via differential S-parameter blocks, so that each port has two terminals (plus/minus). For each port the associated lumped element is placed, either using the predefined capacitor/inductor/resistance blocks or self defined lossy element blocks, to account for losses within the RF coil. These self defined blocks make use of the predefined lumped element blocks. The connection between the 3D EMS and the RF co-simulation side is depicted in Fig. 3.4.

![Figure 3.4: Connection from 3D EM simulation to RF co-simulation. On the left an RF coil model as used in the 3D electromagnetic simulation can be seen. The zoomed-in part depicts a gap for capacitor placement, or in this case a substituted 50 Ω port. In the RF co-simulation (right) all the substituted ports are replaced by the respective lumped element. In this figure the lumped element used is a capacitor. When all ports are equipped with the suitable lumped element, the RF co-simulation can be started.](image-url)
To incorporate realistic loss effects, a lossy capacitor object was created to be used instead of the predefined capacitors from ADS that can be seen in Fig. 3.4. The schematic for a lossy capacitor is shown in Fig. 3.5. The resistance originates from the solder joints used to connect the capacitor to the coil wire. The value of 0.2 $\Omega$ was taken from measurements in Kumar et al. [69].

\[
\begin{array}{c}
\text{P}_1 \quad 0.2\Omega \quad R \quad C \quad \text{P}_2 \\
\end{array}
\]

**Figure 3.5:** ADS lossy capacitor schematic.

### S-parameter simulation

The S-parameter simulation yields a new S-parameter matrix with lumped elements instead of 50 $\Omega$ ports. This result reflects what can be observed on the network analyzer when the RF coil is plugged in. To get an idea of the starting capacitor values, it suffices to approximate the inductance given by the wire length, shape and cross-section, empirical expressions can be found online, e.g [75]. The necessary capacitance value is calculated according to \( \omega = 1/\sqrt{LC} \). This is only an approximation, because the load impedance presented to the coil and the exact losses are not precisely known, but represents a valid starting point for optimization algorithms. As an example, the result of such an initial guess for a three element \(^1\)H array at 3 T can be seen in Fig. 3.6 on the left.

![Reflection parameters for a three channel \(^1\)H coil (3 T).](image)

**Figure 3.6:** Reflection parameters for a three channel \(^1\)H coil (3 T). The untuned condition with guessed capacitor values (left), and the automatically tuned and matched S-parameter plot (right) is shown. The blue line indicates the desired resonance frequency (123 MHz).

ADS offers the possibility of parameter optimization with a number of implemented numerical algorithms. In case of a typical S-parameter simulation for an RF coil, the optimization goals are chosen to minimize the reflection and/or transmission coefficients to
3.2. Numerical Implementation

a certain value. For Fig. 3.6 (right), this was set to minimize $S_{11}$, $S_{22}$, and $S_{33}$ until all values have reached -40 dB. The same concept can be applied for decoupling of coil channels. This procedure corresponds to the tuning and matching stage at the bench. The variables that could be changed to achieve this goal were the capacitor values.

**AC simulation**

Once the coil is tuned and matched, the resulting scaling factors have to be calculated. These scaling factors are used to correct the prototype 3D fields obtained with the FDTD simulation, to correspond to the behavior of the tuned and matched RF coil. For this purpose the electromotive force ($\xi$) for each port is derived according to eq. (2.3.28). The simulation mode is changed to *AC simulation*, now with an AC power source (P_AC) inserted for each coil channel’s feeding port. For the calculation of $\xi$, cross voltages and output currents of the individual lumped elements have to be monitored. This can be realized using available current probes (I_probe) and calculating the voltage as $V_{out} - V_{in}$. This is done for each channel separately, while the other channels are terminated by 50 Ω resistance, to be able to calculate the individual $E$ and $B$ fields for each channel.

The variables that are passed to the post-processing step are

- $k \times k$ S-parameter matrix
- $n$ electromotive force values (*scaling factors*)
- $m$ lumped element cross voltages and output currents

where $k$ is the number of channels, $n$ denotes the total number of ports defined in the FDTD simulation, and $m$ is the number of lumped elements without counting the feeding AC power sources.

### 3.2.3 Post-processing

In this work, the post-processing of the simulated data was performed in Matlab. As input the $E$ and $H$ fields obtained from the FDTD simulation plus the scaling factors (ScF) from the RF circuit co-simulation are used. Before combining the data, the electromagnetic fields from the 3D EM simulation are saved for each defined port ($n$ ports). The fields are combined by multiplying the scaling factors with the prototype fields

$$H_j = ScF_{j,n} \cdot H_{n,(x,y,z)} \quad (3.2.1)$$

where $j$ denotes the respective coil channel, $n$ is the number of ports/scaling factors. The result of this multiplication is the magnetic field produced by coil channel $j$. The same method is applied to the $E$ field to yield the respective coil channel’s electric field.

For evaluation and optimization of an RF coil’s performance, we are interested in the $B_1^+$ (for transmit), the $B_1^-$ (for receive), and the $E$ field. $B_1^+$ and $B_1^-$ can be straight-forward
calculated according to eqn. (??) and (??), remembering that \( B = \mu_0 H \). Since we are working in the respective frame of reference, the term \( e^{\pm i\omega t} \) can be dropped, yielding the following simplification

\[
B_i^+ = \frac{B_{ix} + i \cdot B_{iy}}{2} \quad \text{(3.2.2)}
\]

\[
B_i^- = \frac{(B_{ix} - i \cdot B_{iy})^*}{2} \quad \text{(3.2.3)}
\]

The \( E \) field is used to calculate the local and global SAR. In the following section some optimization figures of merits to optimize and evaluate an RF coil will be presented. What specific figure is used strongly depends on the application.

### 3.2.4 Optimization & Evaluation Procedures

In the theory section we have noted that the transmit field is dependent on the positively rotating magnetic field (\( Tx \propto B_i^+ \)) and the receive field on the negatively rotating field (\( Rx \propto B_i^- \)). In a standard transceive RF coil both sides should be taken into design considerations.

**Transmit**

The total \( B_i^+ \) field used to excite the spins, is the result of combining the individual channel’s fields (\( B_{ij}^+ \)) including amplitude and phase information:

\[
B_{i\text{coll}}^+ = \sum_j e_{v_j} \cdot B_{ij}^+ \quad \text{(3.2.4)}
\]

where \( e_{v_j} \) denotes the excitation parameters of channel \( j \), given as

\[
e_{v_j} = a_j \cdot e^{i\varphi_j} \quad \text{(3.2.5)}
\]

with \( a_j \) being the amplitude and \( \varphi_j \) the phase of excitation for channel \( j \).

Most MR scanners have only one transmit channel per plug. Systems equipped with so-called parallel transmit (pTx) hardware, have more than one transmit channel per plug and are able to supply different amplitudes and phases to each transmitting element. For the application of an RF coil array with a standard scanner, i.e. only one transmit channel is available, the transmit power is split in order to feed all array elements. This is commonly done with power dividers (see section 2.2.7). In an RF coil array different relative phases and amplitudes of transmitting elements have a strong influence on the produced \( B_i^+ \) field (see Fig. 3.7). Changing amplitudes and phases during the transmit phase of a scan is the basic idea of pTx, and sometimes is called dynamic \( B_i^+ \) shimming.

Since the method of parallel transmit is not covered in this thesis, we will focus on the far more common practice of static \( B_i^+ \) shimming. Static \( B_i^+ \) shimming is realized by choosing
a fixed set of amplitudes and phases for each transmitting channel. Conventionally, the amplitudes are kept equal, while the phases are relatively changed against one another by adjusting the cable length. Therefore a useful optimization parameter is the phase difference between respective channels.

\[ \Delta \varphi : -90^\circ -45^\circ 0^\circ +45^\circ +90^\circ \]

Figure 3.7: Produced \( B_1^+ \) field of a two channel \(^1\)H coil, conformed to the lower half of a cylinder at 297.2 MHz (7 T). Depending on the phase difference (\( \Delta \varphi \)) of the input pulse of the two channels, the superposition which forms the total \( B_1^- \) field changes significantly.

When searching for the optimal phase, we first have to define what \textit{optimal} means in the current case. Some common \textit{optimality measures} are listed below

- **Transmit efficiency**, defined as the mean \( B_1^+ \) in some ROI over the square root of absorbed power \( P_{abs} \)
  \[
  TxE := \frac{\overline{B_1^+}}{\sqrt{P_{abs}}} \tag{3.2.6}
  \]

- **SAR efficiency**, defined as the mean \( B_1^+ \) in some ROI over the square root of the maximal local 10 g SAR value in the whole sample
  \[
  SE := \frac{\overline{B_1^+}}{\sqrt{\text{max}(\text{SAR}_{10g})}} \tag{3.2.7}
  \]

- **Relative inhomogeneity**, defined as the standard deviation of the \( B_1^+ \) field in some ROI over the mean \( B_1^+ \) in the same ROI
  \[
  RI := \frac{\text{std}(B_1^+)}{\overline{B_1^+}} \tag{3.2.8}
  \]

- **Combination function** defined to combine relative inhomogeneity and SAR efficiency, yielding one optimality measure,
  \[
  f := \frac{SE}{\text{max}(SE)} \cdot \left( 1 - \frac{RI}{\text{max}(RI)} \right) \tag{3.2.9}
  \]

Without loss of generality, the phase of one channel can be assumed fixed to e.g., 0°. For the remaining \( j - 1 \) channels, phases are varied in increments \( h \), resulting in \( (360/h)^{j-1} \) phase combinations. For each of these, the selected optimality measures are calculated. The optimal phase combination can then be directly obtained from the matrices as the maximum (TxE, SE, and f) or the minimum (RI) value. Fig. 3.8 shows the four optimization matrices obtained for a three channel array. The figures are scaled from worst to best, the optimal phase values are marked with a white circle.
3. RF Coil Development Workflow

Figure 3.8: Optimization matrices, $\varphi_2$ (y-axis) vs. $\varphi_3$ (x-axis) for a three channel array. Each figure of merit (Transmit efficiency ($\text{TxE}$), SAR efficiency ($\text{SE}$), relative inhomogeneity ($\text{RI}$), combination function ($f$)), yields a slightly different optimum in terms of channel phases. The optima are marked with a white circle in each plot.

Receive

In section 2.2.2.1, a relationship between SNR and coil efficiency ($\eta$) was established. This is used to derive a figure of merit ($\mu$) that is proportional to SNR. The coil efficiency (eq. (2.2.31)) can be calculated as [31]:

$$\mu^2 = \eta = \frac{\mathbf{I}^H \mathbf{B}_t \mathbf{B}_t^T \mathbf{I}}{2 \mathbf{I}^H \mathbf{R} \mathbf{I}}$$  (3.2.10)

where $\mathbf{I}$ is a maximize-able column vector representing the currents in each element of the array, $\mathbf{R}$ is the resistance matrix, defined as the real components of the impedance matrix, and $\mathbf{B}_t$ is a matrix containing the $B_1$ magnetic field values at specific points in space for all individual channels, assuming we drive them with 1 A input current. This $\mu$ is very helpful when comparing different coil designs for receive performance rather than deriving actual SNR values.

Example: A three channel $^3^1$P array at 7 T was investigated (see. chapter 4) using the optimization techniques described. The resulting $\mathbf{B}_t^+$, SNR, and SAR distribution for the optimized array can be seen in Fig. 3.9. The $\mathbf{B}_t^+$ field was calculated with an input power of $P_{\text{in}} = 1$ kW and a phase setting of $(66^\circ, 0^\circ, -63^\circ)$, the SNR map was calculated according to eq. (4.3.4). The SAR map is depicted as a maximum intensity projection along the z-axis with an input power of $P_{\text{in}} = 1$ W.

3.2.5 Comparison of different coil designs

The goal of most coil developments is to devise and manufacture a design that functions superior to existing ones. Therefore, different designs are compared already in simulation to establish differences, which is of course dependent on the application of the coil. The following example shall demonstrate how, depending on the figure of merit used to establish meaningful differences, diverging the conclusion of a particular comparison can be.
3.2. Numerical Implementation

Figure 3.9: The $B_1^+$ distribution map (left) was calculated for an input power of 1 kW. The SNR map (middle) was calculated according to eq. (4.3.4) and is proportional to the maximum achievable SNR. The SAR map (right) is a maximum intensity projection along $z$, calculated for an input power of 1 W.

Example: The results of a thorough simulatory comparison of 4 different transceive RF coil designs, which were partly published in [4] and shown in chapter 4, are elaborated in more detail here.

The intended application of the four designs is $^{31}\text{P}$ spectroscopy in the human gastrocnemius and soleus muscle during exercise. Therefore, an optimal design for the lower half of a cylindrical phantom is desired. The geometric description of the designs is given below and can be seen in Fig. 3.10; $r$ denotes the radius of the bending curvature around the calf, $h$ is height, and $l_t$ and $l_e$ is total length and single element length, respectively.

1. Form fitted single loop coil ($r = 7.45 \text{ cm}$, $h = 10 \text{ cm}$, $l_t = 19.2 \text{ cm}$)
2. Form fitted 3 element array with shared conductor ($r = 7.45 \text{ cm}$, $h = 10 \text{ cm}$, $l_e = 6.4 \text{ cm}$, $l_t = 19.2 \text{ cm}$)
3. Small birdcage coil with dimensions as design 2 ($r = 7.45 \text{ cm}$, $h = 10 \text{ cm}$, 16 leg high-pass)
4. Commercially available birdcage coil for $^{31}\text{P}$ studies in the leg ($r = 9 \text{ cm}$, $h = 20 \text{ cm}$, 16 leg high-pass)

Figure 3.10: RF coil model schemes, the leg phantom is depicted as a light blue cylinder, the coil conductors are orange, capacitors are black, and the central slice used for the depicting the figure of merits used in the following comparisons is marked in light green.
There is no explicit standard how to compare different coil designs, therefore appropriate measures have to be identified first. In the following four such figure of merits are stated, each one individually being meaningful for different conclusions.

**Figure of merit 1: \( \frac{B_1^+}{\sqrt{P_{\text{abs}}}} \)**

For a transmit comparison the produced \( B_1^+ \) for all coils is evaluated. Since the designs differ in geometry, size, and type (volume vs. surface coils), and therefore exhibit differently pronounced power balances (reflected, radiated, dissipated power), it makes sense to compare the \( \frac{B_1^+}{\sqrt{P_{\text{abs}}}} \) rather than the transmit field alone (Fig. 3.11).

![Figure 3.11: The transmit field normalized to the square root of the absorbed power \( \frac{B_1^+}{\sqrt{P_{\text{abs}}}} \).](image)

**Figure of merit 2: \( \frac{B_1^+}{\sqrt{\text{max}(\text{SAR}_{10g})}} \)**

Sometimes, and especially in spectroscopic applications, the maximum SAR value is the main limitation of the RF coil. In this case the \( \frac{B_1^+}{\sqrt{\text{max}(\text{SAR}_{10g})}} \) field should be evaluated (Fig. 3.12).

![Figure 3.12: The transmit field normalized to the square root of the max 10 g SAR value \( \frac{B_1^+}{\sqrt{\text{max}(\text{SAR}_{10g})}} \).](image)
3.2. Numerical Implementation

Figure of merit 3: $B_1^+$ per maximum permissible power

When comparing different coil type like surface to volume coils, the safety relevant limitations concerning SAR are different (see Tab. 2.6). To obtain an accurate comparison that is applicable in reality, we should estimate the $B_1^+$ field produced with the maximum permissible input power, which is the forward power (cf. Fig 2.39). For the determination of the maximum permissible power for the four different designs, different safety regulations apply [37]. For surface coils the limiting threshold is that any 10 g tissue subvolume may not exceed a specific absorption rate of 20 W/kg for extremities. For this purpose the k-factor, defined as the maximum $\text{SAR}_{10g}$ value for 1 W input power, is calculated. Volume coils are limited by the exposed body mass, where the exposed mass is defined as the mass where 95% of the power is dissipated. The permissible power calculation can be seen in Tab. 3.2.

<table>
<thead>
<tr>
<th></th>
<th>single loop array</th>
<th>small birdcage</th>
<th>birdcage</th>
</tr>
</thead>
<tbody>
<tr>
<td>k-factor</td>
<td>1.3</td>
<td>1.6</td>
<td></td>
</tr>
<tr>
<td>exposed mass</td>
<td>≈ 2 kg</td>
<td>≈ 3 kg</td>
<td></td>
</tr>
<tr>
<td>total mass</td>
<td>80 kg</td>
<td>80 kg</td>
<td></td>
</tr>
<tr>
<td>safety regulation</td>
<td>20 W/kg</td>
<td>10 W/kg $- (8 \text{W/kg} \cdot \frac{\text{exposed mass}}{\text{total mass}})$</td>
<td></td>
</tr>
<tr>
<td>permissible power</td>
<td>15.4 W</td>
<td>12.8 W</td>
<td>19.6 W</td>
</tr>
</tbody>
</table>

Table 3.2: Maximum permissible power determination. Depending on the type of the coil, i.e. surface or volume, different safety regulations apply. For surface and volume coils the k-factor and the exposed tissue mass, are the limiting factors, respectively.

The $B_1^+$ produced with the individual maximum permissible power can be seen in Fig. 3.13.
Figure of merit 4: SNR

As previously mentioned, for a transceive coil it is important to take the receive performance into account by calculating $\mu$ (eq. (4.3.4)) for each design. Fig. 3.14 shows higher achievable SNR for the array coil in the lower half of the cylindrical phantom.

![Figure 3.14: Optimal SNR in terms of $\mu$](image)

Conclusion of the comparison

From these comparisons, the following conclusions can be drawn:

- as by design, the array (2) is only useful in the lower half of the leg cross-section
- the array (2) outperforms all other designs in receive sensitivity
- the smaller birdcage (3) outperforms the larger one (4) both in transmit and receive performance
- the array exhibits a superficially stronger, but overall more inhomogeneous $B_1^+$ pattern than the small birdcage (3)

Therefore, in the case of studies focused on the investigation of gastrocnemius and soleus muscles, which are located in the lower half of the leg, the array design would be selected.

### 3.3 Hardware Implementation

When a final design is chosen with the help of simulation, a first prototype of the RF coil is built in the lab. Typical tools are used for cutting and bending of conductors, and soldering. Some coil designs can be readily printed or etched. In most cases the RF coil has to be tuned by changing the values of capacitors. Some designs are already printed resonant at the needed resonance frequency, i.e. [76]. However the RF coil is constructed, tuning and matching has to be evaluated for different loading conditions, and possibly adjusted.

To assess the performance of an RF coil, four key parameters can be defined: the $B_1$ field strength and homogeneity, and the losses in the coil and sample, respectively. Although
there are methods for direct measurement of the magnetic field produced by the coil [77], they are difficult to perform on the bench. Therefore $B_1$ field performance is primarily evaluated using simulation techniques. The exact evaluation of losses in the real coil and sample is more accurately measured on the bench compared to simulation, and can be easily done by measuring the Q-factor.

### 3.3.1 Coil construction and choice of materials

When constructing the coil, the engineer has to decide on certain materials that will be utilized in the RF coil design. Typically it is of crucial interest to keep the losses within the used materials low (cf. section 2.3.5). Depending on the function of the component, there are different requirements on the material. In the following paragraphs some considerations and recommendations are listed, concerning the materials used.

**Conductor**

In general any electrically conducting material can be used to form the conductor of an RF coil. To minimize losses, the material should have a very small resistivity ($\rho$), which is a measure of how strong a material opposes the flow of electric current and is measured in $\Omega \text{m}$. Superconductors have a resistivity of 0 $\Omega \text{m}$, metals approximately $10^{-8}$ $\Omega \text{m}$. Most RF coil structures are constructed of copper, which has a resistivity of $1.72 \times 10^{-8}$ $\Omega \text{m}$ [78].

Additionally to the low loss material choice, the geometry of the conductor may have an influence on the suitability of the conductor. There exist various kinds of copper which might be useable for an RF coil, the two most common types are wire, and tape or foil. They are composed of the same material, i.e. copper, and differ only in the geometric shape. Copper tape has many advantages, one being that it can be more easily adapted to any rounded structure, very often it already possess an adhesive side for this purpose. But we have to keep in mind that the effective resistance $R$ of a conducting wire is inversely proportional to its cross-sectional area $A$ [7]:

$$ R = \frac{\rho l}{A} $$

where $l$ denotes the length of the conductor. Copper foil has a thickness of about 18 $\mu\text{m}$ - 35 $\mu\text{m}$, whereas copper wire usually employed in RF coils for MRI has a diameter of 1.5 mm - 3 mm. Therefore we anticipate higher losses due to increased resistance in the copper tape.

At higher frequencies the effective resistance of conductors increases due to the skin effect. The skin effect represents the tendency of alternating current to form a distribution such that the current density is highest close to the surface of the conductor. This greatly reduces the cross-sectional area of the conduction, which increases the effective resistance.
to alternating current (see eq. (3.3.1)). This effect increases with frequency [5, 79], which can be seen in Fig. 3.15. For copper, the skin depth at 100 MHz is approximately 6.6 µm.

\[ \delta \]

\[ d \]

\[ \sigma \]

\[ \delta \]

\[ d \]

Low frequency

High frequency

Figure 3.15: Skin effect in wire with diameter \( d \). The skin depth \( \delta \) decreases with increasing frequency. The conducting area is depicted in blue.

Kumar et al. [69] calculated the effective resistance and skin depth for copper wire and copper strip loops, tuned to the same four resonance frequencies (49 MHz, 64 MHz, 124 MHz, 207 MHz), and concluded that there is no significant difference in the skin depth or effective resistance originating from the copper type used. They also investigated the noise figures (NF) for single and array loops, constructed of copper wire and flat copper stripes, and concluded that the NF is better for coils that are tuned with 2 than 4 capacitors. No differences due to the copper type could be established. However, they also observed an increase in the NF for the flat strip overlap coil array when the number of elements increases (see [69, Fig. 5]).

In conclusion, in order to minimize coil losses, especially in overlap arrays, the use of copper wire is evident. However, it should be mentioned that when operating in the sample loss regime (cf. section 2.2.4), the coil loss minimization due to the choice of conductor type may be negligible.

### Capacitors

The capacitors that are employed in RF coil design to tune, match, and possibly decouple the coil, should obviously be MR compatible, i.e. non magnetic capacitors. Capacitors can be chosen to have a fixed value, with a certain tolerance level which depends on the quality of the capacitor and the fabricator. Additionally to fixed capacitors there exist adjustable capacitors (trimmers), which cover a specific range of capacitance values. When choosing the capacitors, one should turn one’s attention to the capacitors Q-factor and in case of a transmit coil, its working voltage range. When capacitors are supplied with voltages
above its working voltage limit, it can either break or electric sparks are generated. Both
scenarios change the RF coils characteristics either permanently (break down), or during
the measurement (sparking), potentially introducing danger to the patient/volunteer. The
Q-factor and the voltage range can be determined from the data-sheet of the respective
capacitors. Unfortunately, the working voltage is usually given for direct current, not
alternating current as is the case in MR RF engineering. Therefore, we identified two
tests that can be used to investigate the working range of the capacitors. The tests are
described in section 3.4.3.

Housing

The resonant circuit as the assembly of conductors and capacitors has to be placed inside
a housing. When in vivo measurements are planned it is advisable to use some kind
of opaque material to hide the electric circuit from the patient or volunteer. Since the
housing is usually very close, even touching the circuit, one has to pay attention on
the dielectric properties of the material. The dielectric losses occurring in a dielectric
material, can be described by the loss tangent $\tan(\theta)$, where $\theta$ denotes the loss angle. The
complex permittivity can be written in terms of its real and imaginary part: $\varepsilon_d(\omega) =
\varepsilon'_d(\omega) + i\varepsilon''_d(\omega)$. Then the loss tangent is defined as [79]

$$
\tan \theta = \frac{\sigma_c(\omega)}{\omega\varepsilon'_d(\omega)} + \frac{\varepsilon''_d(\omega)}{\varepsilon'_d(\omega)} \tan \theta_d
$$

(3.3.2)

where $\omega$ is the angular frequency, and $\sigma_c(\omega)$ is the real-valued, frequency dependent
electrical conductivity. In the equation above, the total loss tangent can be interpreted
as the sum of two loss tangents, namely $\tan \theta_c$ describes the losses due to conduction,
and $\tan \theta_d$ are the losses due to polarization. In the lossless case, the loss tangent is 0.
When deciding on the material, is loss tangent close to 0 is the favorable choice. Table
3.3 states the loss tangent of some common materials used for coil housing\textsuperscript{1}.

<table>
<thead>
<tr>
<th>Material</th>
<th>Loss tangent @ 100 MHz</th>
<th>Loss tangent @ 10 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Teflon (PTFE)</td>
<td>0.0002</td>
<td>0.00015</td>
</tr>
<tr>
<td>Polystyrene, glass microfiber</td>
<td>0.0004</td>
<td>0.002</td>
</tr>
<tr>
<td>ABS</td>
<td>0.005</td>
<td>0.019</td>
</tr>
<tr>
<td>Pyrex glass</td>
<td>0.003</td>
<td>0.007</td>
</tr>
<tr>
<td>PolyEthylene, DE-3401</td>
<td>0.0002</td>
<td>0.00031</td>
</tr>
</tbody>
</table>

Table 3.3: Loss tangents measured at 100 MHz and 10 GHz for some commonly used materials
in RF engineering.

\textsuperscript{1}http://cp.literature.agilent.com/litweb/pdf/genesys200801/elements/substrate_tables/tablelosstan.htm
In addition, bio-compatibility of the housing material is of importance when the coil will be used in a clinical setting. This includes a surface that is easy to clean.

### 3.3.2 Bench testing

During and after construction of the RF coil it is tested in the lab. This is called bench testing. The tool that is by far most often used during this period is the network analyzer.

**Network Analyzer**

The bench measurements are mainly performed on a network analyzer (NWA). The NWA enables the measurement of amplitude and phase information of electrical networks as a function of frequency. A typical NWA consists of a signal generator, generating a test signal which is routed to the circuit under investigation, also called device under test (DUT), by a signal-separation device (SSD). The SSD also routes the altered signal to the receivers (at least one) where the signal is detected. Finally there is a processing and displaying unit for calculating and reviewing the results.

**S-parameters**

The measured quantity are the scattering parameters (S-parameters), i.e. the incident, reflected and transmitted waves, of the electrical networks under test (see Fig. 3.16). S-parameters are complex, linear quantities. For some measurements it is favorable to express them in a logarithmic magnitude format, to have a higher dynamic range than choosing a linear magnitude display.

\[
S_{ij} \text{ [dB]} = 20 \cdot \log_{10}(S_{ij} \text{ [lin]}) \tag{3.3.3}
\]

**Figure 3.16:** Schematic of a two port NWA measurement. The incident wave into port 1 is denoted \( a_1 \), the reflected wave is \( b_1 \) and the signal transmitted to 2 is denoted \( b_2 \).

For an \( n \)-port circuit, the S-parameter matrix or S matrix is a symmetric \( n \times n \) matrix defined as

\[
b = Sa \tag{3.3.4}
\]

where the vector \( b \) stands for the outgoing waves, and \( a \) for the incident waves. The in-and outgoing waves are defined in terms of voltages and currents:

\[
a_1 = \frac{V_1 + Z_0 I_1}{2 \cdot \sqrt{Z_0}} \quad a_2 = \frac{V_2 - Z_0 I_2}{2 \cdot \sqrt{Z_0}} \tag{3.3.5}
\]

\[
b_1 = \frac{V_1 - Z_0 I_1}{2 \cdot \sqrt{Z_0}} \quad b_2 = \frac{V_2 + Z_0 I_2}{2 \cdot \sqrt{Z_0}} \tag{3.3.6}
\]
where \( Z_0 \) denotes the characteristic impedance. In case of transmitting with port 1 only, i.e. \( a_2 = 0 \), the S matrix is given by

\[
S_{11} = \frac{b_1}{a_1} \quad S_{12} = S_{21} = \frac{b_2}{a_1}
\]

(3.3.7)

The diagonal elements of the S matrix are the reflection coefficients, and offer information about the resonance of an electrical circuit, i.e. at the resonance frequency the reflection coefficients exhibit a notch (see Fig. 3.17, red and yellow curve), because at resonance energy is dissipated in and radiated by the resonant circuit. The off-diagonal elements are called transmission coefficients. In case of an \( n \) element system, the parameter \( S_{ij} \) describes the transmission from port \( j \) to port \( i \). The transmission coefficients give information about the decoupling performance of individual coil elements (see Fig. 3.17, green curve).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{s-parameter_plot.png}
\caption{Log-Mag S-parameter plot of a two channel RF coil array for \( ^{31}\)P spectroscopy at 7 T (120 MHz, blue line). The untuned and unmatched situation is depicted in (a), both channels resonate close to, but not exactly at the desired Larmor frequency. After tuning and matching (b) the two channels strongly couple with one another, resulting in a resonance peak splitting. After decoupling, the resonance peaks equal the Larmor frequency again, coupling between elements is still present.}
\end{figure}

**Q-factor measurement**

The network analyzer should have the characteristic impedance of the MR scanner, i.e. 50 \( \Omega \). In this case the coil can be plugged directly to the analyzer since it already has to be matched to the necessary 50 \( \Omega \) impedance of the system. When the coil is not sufficiently matched, the S-parameter measurement is biased due to heavy reflection. In such circumstances, a sniffer loop can be used for measurements of the Q-factor. The sniffer loop is connected to the analyzer and couples weakly with the resonant structure, therefore offering information about the RF coil. Sniffer tools consist of either one or two loops [77, 80]. In case of a double loop, the two loops have to be decoupled from each other, e.g. using overlap or orthogonal positioning (see Fig. 3.18). Then each loop is connected to one port and the transmission coefficient (\( S_{21} \)) is measured. The transmitting
loop induces a current in the RF coil, which on the other hand induces a voltage in the second sniffer loop. The $S_{21}$ curve will show a dip at the resonance frequency of the RF coil.

![Sniffer Loop designs](image)

*Figure 3.18: Sniffer Loop designs*

Equation (2.2.47) showed that the Q-factor can be calculated as the ratio of the frequency of the $S_{21}$ curve’s local extremum (i.e. at the resonance frequency) to its -3 dB bandwidth.

\[
Q = \frac{\omega_0}{\Delta \omega_0}
\]  

(2.2.47)

Care must be taken that the sniffer loops couple only weakly to the resonator (<-40 dB), to avoid dampening of the frequency response [40].

It is possible to measure the Q-factor by means of the frequency response of the reflected signal when the coil is directly connected to the NWA. This measurement yields half of the quality factor and is only valid in case of perfect matching [40].

An exemplary Q-factor measurement for a single $^1$H RF coil for 7 T can be seen in Fig. 3.19. For the measurement a double sniffer loop with overlap decoupling was used. The figure shows the $S_{21}$ parameter measured with a network analyzer (E5061B, Agilent, Santa Clara, USA). From the narrow peak (i.e. the small bandwidth), it can be seen that the Q-factor of the unloaded coil is much higher than that of the loaded coil. Additionally, a slight shift of the resonance frequency ($\approx 3$ MHz) is observed when the coil is loaded with a sample. The respective Q-factors can be calculated as

\[
\begin{align*}
Q_u &= \frac{296.78}{120} \approx 247.32 \\
Q_l &= \frac{299.71}{24.97} \approx 12.00
\end{align*}
\]

$$Q_u \approx 20.61$$  

With a Q-ratio of $\approx 20.605$ the coil operates well within the sample noise regime (see equation (2.2.49))
3.4 MR Performance

Once the RF coil is physically built, its functionality is tested inside the scanner. Additionally there are procedures to verify the simulation results.

To yield realistic and comparable results, a tissue-like phantom has to be used for MR experiments. In this thesis the phantoms used for MR measurements were fabricated according to the ASTM standard "F2182-11A, Standard Test Method for Measurement of Radio Frequency Induced Heating On or Near Passive Implants During Magnetic Resonance" [81]. Care must be taken to obtain the correct tissue parameters, especially electrical conductivity (\(\sigma\)). To alter \(\sigma\), NaCl is added to the solution until the conductivity value is reached. To achieve a physiological \(^{31}\text{P}\) concentration, 30 mM of KH\(_2\)PO\(_4\) was added during the gel production, to enable testing the \(^{31}\text{P}\) part of the developed RF coils.

3.4.1 \(B_1^+\) Mapping

To test the performance of the RF coil, and to validate the magnetic field simulations, the transmit field (\(B_1^+\)) can be visualized with the help of the MR system. There are numerous techniques enabling accurate mapping of the \(B_1^+\) field [82]. The available techniques can be roughly divided into two groups: image-based and phase-based, both groups include techniques working in the 2D or 3D regime. Most methods use the magnitude/phase information obtained by combining two images to form a third.

The \(B_1^+\) field cannot be directly detected with MR imaging methods, but the flip angle distribution can be. The relation of these two entities is shown in Fig. 2.5c and eq. (2.1.27), confirming that the actual flip angle achieved by an RF pulse is dependent on
the pulse duration ($\tau$), the gyromagnetic ratio, and the $B_1^+$ field. For an arbitrary RF pulse of shape $f(t)$ it can be described by

$$\alpha(x) = \gamma B_1^+(x) \int_0^\tau f(t) dt$$  \hspace{1cm} (2.1.27)

This flip angle distribution can be mapped with the MR system and then related to the $B_1^+$ distribution with the knowledge of pulse shape and duration.

Due to its simplicity, the gold standard for $B_1^+$ mapping is the so called double angle method (DAM), firstly published in 1993 by Insko et al. [83]. The signal obtained by an MR experiment employing a pulse that results in an flip angle of $\alpha$ is proportional to

$$S \propto M_0 \sin(\alpha)$$  \hspace{1cm} (3.4.1)

The double angle method uses the trigonometric identity of $\sin(2\alpha) = 2\sin(\alpha)\cos(\alpha)$ to calculate flip angle maps, by acquiring two images ($S_1$, $S_2$) with nominal flip angles $\alpha_1$ and $\alpha_2 = 2\alpha_1$. Calculating their ratio yields

$$\frac{S_1}{S_2} = \frac{M_0 \sin(\alpha_1)}{M_0 \sin(\alpha_2)} = \frac{2\sin(\alpha_1)\cos(\alpha_1)}{\sin(\alpha_1)} = 2\cos(\alpha_1)$$  \hspace{1cm} (3.4.2)

Then $\alpha_1$ can be easily obtained by calculating

$$\alpha_1 = \arccos\left(\frac{S_2}{2S_1}\right)$$  \hspace{1cm} (3.4.3)

Care must be taken to avoid $T_1$ dependency in the acquired images by using a repetition time of $TR > 5T_1$, which typically results in very long scanning time. Also, only flip angle variations of $0^\circ < \alpha < 90^\circ$ can be successfully mapped with one DAM run. To map flip angles from $0^\circ$ – $180^\circ$ though, the method can be extended to use the phase information [84]. To get rid of the $T_1$ dependency, it is advisable to use saturation pulses, as proposed in [85].

**Example:** Two channel 7 T proton coil for calf muscle studies. The measured flip angle (FA)/$B_1^+$ and simulated $B_1^+$ maps can be seen in Fig. 3.20, showing very good agreement qualitatively and quantitatively. The $B_1^+$ map was calculated from the flip angle (FA) map according to equation (2.1.27).

### 3.4.2 Temperature Mapping

In the previous section, a technique of experimentally mapping the magnetic field produced by the coil was introduced. However, the agreement of simulation and measurement of the magnetic field unfortunately does not automatically imply the same for the electric field and SAR distribution. Since SAR, due to the relevant legislation, is the main safety measure in MRI and MRS protocols today, it would be favorable to have a method to
3.4. MR Performance

Figure 3.20: The measured and simulated $B_1^+$ maps of a two channel $^1$H array for calf muscle studies can be seen this figure. The maps agree in both distribution and magnitude.

Experimentally evaluate the simulated results, much like for the transmit field. There exist detailed guidelines on how much energy may be deposited in the body while ensuring safe use [37]. But what actually may harm the patient is not the E-field nor SAR itself, but the resulting heating of the tissue. There exist several methods to map temperature changes indirectly from changes in the MR signal [86].

3.4.2.1 Temperature and SAR

Since the SAR distribution from an RF coil is related to the temperature distribution, the simulation can be indirectly verified. The temperature change due to effects of thermal conduction, perfusion, metabolism, and heat absorption, in tissue can be modeled using Pennes bioheat equation [87]:

$$\rho c \frac{dT}{dt} = \nabla \cdot (k \nabla T) + (\rho_{\text{blood}} w c_{\text{blood}} (T - T_{\text{core}})) + Q_m + \text{SAR} \cdot \rho$$  \hspace{1cm} (3.4.4)

where $\rho$ is the respective material density, $c$ the heat capacity constant of the respective medium, $T$ denotes the temperature in K, $k$ is the thermal conductivity, $w$ represents the perfusion by blood, $Q_m$ accounts for the heat generated by metabolism, and $t$ is time. In case of a phantom we can safely assume it to be a non-perfused material without metabolic heating, hence the temperature change is given by

$$\rho c \frac{dT}{dt} = \nabla \cdot (k \nabla T) + \text{SAR} \cdot \rho$$  \hspace{1cm} (3.4.5)

In order to directly relate the SAR to $dT/dt$, the heat conduction term has to be negligible. At thermal equilibrium, this is indeed the case for a short time after SAR initialization, because thermal conduction requires time to significantly effect the temperature distribution.
To estimate the period of time where thermal conduction is negligible, a preliminary experiment is conducted. With the use of non-magnetic fiber optic temperature probes, it is possible to measure absolute temperature inside the magnet. The probes are placed at two different locations within the phantom (e.g., Fig. 3.21a), one where high SAR/temperature rise is anticipated, and the other one where no significant SAR is expected. The RF coil, as the only heating source, is used to achieve a measurable temperature increase in the phantom.

**Example:** As an example, the temperature increase experiment used for the calf coil described in section 4 can be seen in Fig. 3.21. The preliminary test shows that approximately 110 s after initialization of heating the temperature curve starts to flatten (Fig. 3.21b), indicating heat conduction starts to affect the temperature distribution.

![Fig. 3.21](image)

**(a) Positioning of the two probes and the mapping slice.**

**(b) Preliminary temperature increase test.**

**Figure 3.21:** The preliminary temperature increase testing setup to determine the time period where heat conduction is negligible. Two fiber-optic temperature probes measure the absolute temperature (a) close to the coil (Probe 1), and in the middle of the phantom (Probe 2). A linear temperature increase can be observed for the first 110 s after heating initialization, implying no heat conduction significantly alters the temperature distribution.

Hence, as long as heat conduction in negligible, there exists a direct relationship between SAR and temperature change given by

\[
\frac{c\Delta T}{\Delta t} = \text{SAR}
\]  \hspace{1cm} (3.4.6)

This relation can be used to calculate SAR maps out of temperature change maps.
3.4.2.2 Proton Resonance Frequency Shift

A widely used method for temperature mapping is the proton resonance frequency shift (PRF) method [88]. This method is based on the temperature induced phase shift. We have already seen that the exact Larmor frequency of a nucleus is dependent on the chemical environment (eq. 2.1.48). In case of the hydrogen nucleus ($^1$H), electrons of the water molecule are shielding the nucleus from the $B_0$ field. In a free $H_2O$ molecule the hydrogen nucleus is more efficiently shielded than a $^1$H nucleus in a $H_2O$ molecule that is hydrogen bonded to another molecule. These hydrogen bonds in $H_2O$ vary with temperature [89]. With rising temperature the hydrogen bonds change their physical behavior, resulting in an increased electron shielding of the proton nucleus and, thus, a lower magnetic field.

The temperature dependency ($\alpha$) varies approximately linearly with temperature. For pure water it varies about $-1.03 \pm 0.02 \cdot 10^{-8}/^\circ C$ for temperatures in the range of $-15^\circ C$ to $100^\circ C$ [86].

From two GRE phase images, where one is acquired before temperature change ($I_0$) and one after ($I_p$), the relative temperature can be calculated as

$$\Delta T = \frac{\varphi(I_p) - \varphi(I_0)}{\gamma \alpha B_0 T_E}$$

(3.4.7)

where $\varphi(I_p)$ and $\varphi(I_0)$ are the phase informations of the two GREs, $T_E$ is the echo time, and $\alpha$ is the temperature coefficient. The difference in the phase images ($\Delta \varphi = \varphi(I_p) - \varphi(I_0)$) resembles the phase change due to temperature increase.

For the temperature mapping protocol for the given example in Fig. 3.21, $\Delta t$ was set to 110 s. The resulting temperature map can be seen in Fig. 4.7 and 3.22(a). The simulated unaveraged local SAR can be seen in Fig. 4.7 and 3.22(b).

![Figure 3.22](image)

Figure 3.22: The figure shows the temperature maps acquired using the PRF method (a), and the simulated unaveraged SAR map. The slice position can be seen in Fig. 3.21a. To ensure comparability the temperature probe measurements were compared to the simulated results. Figure take from [4], with permission.

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Since within the 110 s after initialization of heating, the temperature increase is directly proportional to the unaveraged local SAR (eq. (3.4.6)), those two maps are differing by a factor $c$, which was set to be the heat capacity of water ($\approx 4.2 \text{ J/g/K}$). The measured temperature map is in very good agreement with the simulated SAR map.

### 3.4.3 Stability Testing

As previously described, in transceiver arrays it is very important to use high voltage maintaining, non-magnetic capacitors. When capacitors are supplied with AC voltages above their working voltage range, they might break, resulting in an altered performance of the RF coil. The data sheet of the used capacitors specifies the working voltage range. In an RF coil it is not straight forward to calculate the voltages that are present at each capacitor. Therefore in order to find the real working voltage limit for a specific design, stability tests are conducted.

We defined two tests that help establish the voltage stability. Both tests are conducted inside the MR scanner. The coil is loaded with a phantom, which has a signal generating small sphere ($d = 17.5 \text{ mm}$) inserted. The measurement sequence is a simple FID sequence. Since the only signal generating sample is inside the sphere the received signal is somewhat localized. Fig. 3.23 depicts the setup with the $^1\text{H}/^{31}\text{P}$ calf coil. For testing the voltage stability for the $^{31}\text{P}$ array, the signal generating sphere, which is depicted in green, contains a phosphorus solution, while the rest of the phantom fluid contains only saline to match the loading condition of the coil.

**Figure 3.23:** Scan setup for voltage stability testing for the $^1\text{H}/^{31}\text{P}$ calf coil. The green sphere is filled with a phosphorus solution, while the phantom fluid does not contain any $^{31}\text{P}$. Therefore, the phosphorus signal that is received originates only from this sphere.

#### Test I

In the first test the performance stability over a wide range of pulse voltages is tested. For this purpose, the pulse duration is kept constant for all measurements, and the pulse voltage is varied. The local maxima are achieved with the pulse voltages that produce the $90^\circ$, $270^\circ$, $450^\circ$, ... flip angle. The signal is 0 for the voltages that produce the $180^\circ$, $360^\circ$, $540^\circ$, ... flip angle. The distance between each maximum/minimum should be constant.
Example: The test setup depicted in Fig. 3.23 was used to conduct the described test for the $^{31}$P array. The test was performed with a pulse duration of 2 ms and 200 equidistant measurement points. The maximum used voltage was 224 V. The measured data points were fitted with a quadratic function for each of the following intervals: [0°, 180°], [180°, 360°], [360°, 540°], [540°, 720°], and [720°, 900°]. The measured data points and the corresponding fit can be seen in Fig. 3.24 (left) as red crosses and an orange line, respectively. Fig. 3.24 (right) also shows the discrepancy between the theoretical signal evolution (green, dashed) and the measured one (orange).

![Measured and Fitted Data](image1)

![Reality and Theory](image2)

**Figure 3.24:** Stability test I. The measured and fitted data can be seen in the left. Pulse duration was 2 ms, pulse voltage changed from 2.2 V - 224 V in 200 equidistant steps. Data points in the described flip angle intervals were used to determine the quadratic fit. The discrepancy between reality and theory can be seen on the right. Signal amplitude is decreasing with increasing pulse voltage due to $B_0$ inhomogeneities.

We note that the signal amplitude is decreasing with increasing flip angle, which is due to accumulated relaxation effects that are more visible with higher flip angles. A close match between reality and theory could be observed regarding the position of the null signal and the local maxima. The results of this test suggests good voltage stability for pulses below 2 ms up to a pulse voltage of 224 V. Additional tests are required to cover a wider range of voltage stability, e.g. for longer pulses and even higher voltages. Those tests are not shown here.

**Test II**

The second stability test is conducted to obtain more insight about the reproducibility of a signal amplitude. If a measurement result can not be reproduced with the same measurement parameters, further analysis might fail due to false data. Failing reproducibility can be a sign of voltage instability of the RF system. There are two different implementations of this test. First, determine the area under the pulse (AuP), defined as pulse

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voltage $\times$ pulse duration [V$\cdot$ms], necessary for the 90° pulse. Set up the measurement in order to produce a 45° flip angle. The 45° flip angle in beneficiary in this stability test, since we have a far higher dynamic range there compared to the dynamic range of the signal achieved with a 90° flip angle. Repeat the measurement a certain number of times with the following specifications:

1. not changing any parameters
2. changing pulse voltage [V] and pulse duration [ms], but maintaining the 45° flip angle AuP

Both measurement cycles should yield a constant signal amplitude.

**Example:** Fig. 3.25 shows the result of the described stability test (implementation 2) for the $^{31}$P array of the $^1$H/$^{32}$P calf coil. The test was conducted 3 times with changing position of the signal generating sphere (see Fig. 3.23). The three positions were at 1.5 cm, 3 cm, and 4.5 cm away from the bottom phantom wall. For these distances the area under the pulse to achieve a 45° flip angle were 32 V$\cdot$ms, 51 V$\cdot$ms, and 128 V$\cdot$ms. Pulse duration and voltage was changed for each of the 30 measurement points while keeping the respective AuP constant. The result shows a very stable performance.

![Figure 3.25: Stability test II. At three different positions of the signal generating sphere, and thus for three different values of the area under the pulse (AuP) necessary to achieve a 45° flip angle, the pulse duration and voltage were changed for 30 measurement points to yield a constant AuP for each series. The three series show a good voltage stability over a wide range of pulse durations and amplitudes.](image)

**3.4.4 Noise Correlation Matrix**

The noise correlation matrix ($R_{nc}$) introduced in section 2.2.6.4 can be measured by obtaining noise measurements of each coil element, i.e. the excitation voltage equals zero. For an N element array, the noise correlation matrix, which is a normalized version of the noise covariance matrix, is an $N \times N$ matrix.
First we calculate the noise covariance matrix $\Psi$, where the coefficients are calculated by

$$\Psi_{ij} = \frac{1}{2N} \sum_{k=1}^{N} n_i^*(k)n_j(k)$$  \hspace{1cm} (3.4.8)

Here, $N$ is the number of noise only data samples, $n_i(k)$ is the noise acquired in coil element $i$. The diagonal elements, representing the correlations of noise of the same coil element, of $R_{nc}$ are naturally equal 1. Different loading samples influence the coil as well. For a proper evaluation of the noise correlation it is advisable to measure the noise correlation matrix in each measurement, or use an average over a certain number of previously measured samples.

**Example:** Fig. 3.26a depicts the noise correlation matrix measured, calculated, and averaged over 7 separate measurements. The coil was loaded with a phantom containing $^{31}$P gel.

![Noise Correlation Matrix](image)

(a) Noise Correlation Matrix  \hspace{1cm} (b) Measured SNR map of a 3 channel $^1$H coil at 3 T

**Figure 3.26:** Noise correlation matrix and SNR map. The noise correlation matrix for the 3 channel phosphorus coil is shown in (a). An exemplary SNR map of a 3 channel $^1$H coil at 3 T is shown in (b).

### 3.4.5 SNR maps

In order to estimate the signal to noise ratio of magnitude images acquired with RF array coils, the easiest implementation is a 2-ROI based analysis [91]. A signal free region is chosen where the standard deviation of the noise is calculated and then used to estimate the SNR by using the signal intensities divided by the standard deviation of the noise. It has been shown that the use of array coils together with new reconstruction techniques can influence and falsify the 2-ROI based analysis [92].
Especially in parallel imaging data, the noise varies highly across the image. A fact that is represented by the position dependent g-factor [93], making noise-only-region SNR maps, like the one described above, not suitable for the purpose of evaluating array coils. The principle of how signals from individual elements are combined was already shown in section 2.2.6.4. For choosing the best suited weighting factors, there exist various methods [42, 31, 94, 93, 90].

For the calculation of the signal-to-noise ratio we use a Monte Carlo based method that requires one noise pre-scan and one (possibly accelerated) image acquisition. It is called "pseudo multiple replica" method [90] and can also be used to calculate g-factors in a parallel imaging acquisition.

**Example:** The SNR map acquired with 200 pseudo replicas of a 3 channel proton RF coil array at 3 T loaded with a phantom can be seen in Fig. 3.26b. The $^1$H array is of the same dimensions as the 3 channel $^{31}$P array of the previously mentioned calf coil (see chapter 4). Due to the similar Larmor frequency of $^{31}$P at 7 T, i.e. 120.3 MHz, and $^1$H at 3 T, i.e. 123 MHz, it was possible to use the same array with slight modifications of the capacitor values to adjust the 3 MHz resonance frequency difference.

**Summary**

This chapter presented the developed workflow, which includes 3D EM simulation techniques and evaluation methods inside the MR system. Those evaluation techniques can be used to confirm the simulation findings, as well as to ensure safe use of the developed RF coil.
A Form-Fitted Three Channel $^{31}\text{P}$, Two Channel $^{1}\text{H}$ Transceiver Coil Array for Calf Muscle Studies at 7 T

The following chapter is an exact replica of the paper published as "A form-fitted three channel $^{31}\text{P}$, two channel $^{1}\text{H}$ transceiver coil array for calf muscle studies at 7 T" in Magnetic Resonance in Medicine, July 2014, doi: 10.1002/mrm.25339

4.1 Abstract

Purpose

To enhance sensitivity and coverage for calf muscle studies, a novel, form-fitted, three-channel phosphorus-31 ($^{31}\text{P}$), two-channel proton ($^{1}\text{H}$) transceiver coil array for 7 T MR imaging and spectroscopy is presented.

Methods

Electromagnetic simulations employing individually generated voxel models were performed to design a coil array for studying nonpathological muscle metabolism. Static phase combinations of the coil elements’ transmit fields were optimized based on homogeneity and efficiency for several voxel models. The best-performing design was built and tested both on phantoms and in vivo.

Results

Simulations revealed that a shared conductor array for $^{31}\text{P}$ provides more robust interelement decoupling and better homogeneity than an overlap array in this configuration. A
static $B_1^+$ shim setting that suited various calf anatomies was identified and implemented. Simulations showed that the $^{31}$P array provides signal-to-noise ratio (SNR) benefits over a single loop and a birdcage coil of equal radius by factors of 3.2 and 2.6 in the gastrocnemius and by 2.5 and 2.0 in the soleus muscle.

**Conclusion**

The performance of the coil in terms of $B_1^+$ and achievable SNR allows for spatially localized dynamic $^{31}$P spectroscopy studies in the human calf. The associated higher specificity with respect to nonlocalized measurements permits distinguishing the functional responses of different muscles.

**4.2 Introduction**

Phosphorus-31 ($^{31}$P) spectroscopy strongly benefits from recent advances in ultra-high field MR [95, 96], due to the intrinsically higher polarization, increased spectral resolution, and shorter $T_1$-relaxation times at 7 T [97]. High-energy metabolites in the exercising skeletal muscle are frequently studied in the posterior muscle groups of the calf [98, 99], often using dedicated ergometers [100, 101, 102]. To fully exploit the potential of $^{31}$P MRS at 7 T, however, radio frequency (RF) coil sensitivity, homogeneity of the RF field ($B_1$), and spatial coverage have to be optimized.

Coil sensitivity is a critical factor because an increased signal-to-noise ratio (SNR) may be traded in for higher temporal resolution and/or spatial localization of the signal. Localized single-voxel spectroscopy provides higher tissue and metabolic specificity compared to nonlocalized techniques [101]. The higher specificity can be used to differentiate between the metabolic response of neighboring muscles, for example, between the gastrocnemius medialis and lateralis [103] or soleus muscles [104] in the exercising human calf. Also, chemical shift imaging (CSI) strongly benefits from coil sensitivity because of the inherently lower signal from small voxel volumes. Considerable sensitivity improvement can be achieved also by form-fitting the RF coil geometry to the targeted anatomical area.

Three different types of RF coils are commonly used for $^{31}$P skeletal muscle spectroscopy studies. In most studies, RF coils based on planar single-channel $^{31}$P surface loops [98, 99, 100, 101, 105, 106, 107] were used, usually with an additional single loop tuned to the proton Larmor frequency to allow for shimming of the static magnetic field ($B_0$) and scout imaging. Surface coils show high sensitivity close to the coil, but exhibit an inhomogeneous field distribution and lack the required sensitivity for investigations of deeper lying tissues such as the soleus muscle [105, 108]. Other studies used birdcage-type volume coils [109, 110, 111, 112, 113, 114] benefiting from a more homogeneous $B_1^+$ field at the cost of sensitivity. One of the most prominent approaches to enhance
coil sensitivity is the use of phased arrays [42, 31, 115], commonly employed for $^1$H MRI at all available field strengths, but less often seen in coils for $^{31}$P [116, 117, 118, 119, 120]. Array coils combine the advantages of surface loops and volume coils by offering an extended and more homogeneous coverage compared to single loops and of boosting coil sensitivity compared to volume coils. A challenge in coil array design is the mutual coupling between array elements [42, 115], which can be addressed by inductive and/or capacitive decoupling methods [46, 121].

Regardless of the static magnetic field strength, there is usually no body coil available at frequencies other than the $^1$H Larmor frequency; therefore, all coils for nuclei other than $^1$H (X-nuclei) must be local transmit coils. This can be achieved by either separating transmit and receive coil(s) or by employing transceiver coils driven via transmit/receive (T/R) switches. Due to the demanding requirements for sensitivity and transmit efficiency, and in view of the potential use for parallel transmit systems [45], transceiver RF coil arrays are promising candidates for next generation $^{31}$P coils. Design and safety evaluation of local transmit coils require full wave three-dimensional (3D) electromagnetic (EM) field simulation [122], as well as experimental validation for establishing functionality and safety. The most commonly employed simulation method is the finite difference time domain technique [3], previously used for analysis and optimization of RF coils [36, 123, 124].

In this paper, we describe the design, optimization strategies, and construction of a form-fitted $^{31}$P/$^1$H transceiver coil array, specifically designed for metabolic $^{31}$P studies of exercising human calf muscles at 7 T, for which the gastrocnemius medialis (Gm) and soleus (Sol) muscles are of particular interest [98, 99, 100, 101, 102]. A total of three $^{31}$P channels was chosen to benefit from increased sensitivity compared to a single channel coil, while limiting the drawbacks of higher complexity in postprocessing of spectroscopic data and coil element decoupling. Two $^1$H channels were considered adequate to cover the volume of the calf with sufficient homogeneity. We specifically focus on EM simulation to provide a sound basis for design choices in the construction of this novel RF coil array. Simulation comparisons for different decoupling techniques and RF coil designs, as well as temperature measurements and bioheat simulations, are presented. To demonstrate an application of the coil, in vivo $^{31}$P spectra acquired in the Gm and Sol muscles before and after a plantar flexion exercise task are shown. In this study, the $^1$H array was used for scout imaging and shimming only, but the coil can also be used for sequential acquisition of $^1$H and $^{31}$P signal, as recently described by Schmid et al. [125]. The $^1$H array of this coil can also be used alone, as has been shown for simultaneous perfusion quantification by pulsed arterial spin labeling and $T_2^*$-weighted imaging [126] employing an acceleration factor of 2.
4.3 Methods

Subjects and Phantoms

Five healthy volunteers (3 male, 2 female; age 30 ± 6 yrs; body mass index [BMI] = 22.2 ± 2.6 kg/m\(^2\)) were measured with the new form-fitted array coil. The individual calf circumferences are stated in Table 4.1. Four volunteers were measured for creating the individual voxel models described below, and the fifth volunteer underwent a plantar flexion exercise protocol. The study was conducted in accordance to the Declaration of Helsinki after informed written consent of the volunteers and with the approval of the local ethics committee in compliance with the Austrian Medical Product Act.

For phantom measurements, a gel with tissue-like electrical properties was produced according to the ASTM F2182-11a standard [81]. The phantom consisted of an acrylic glass cylinder with 14-cm outer diameter and a length of 20 cm, filled with a gel containing deionized water; 30 mM KH\(_2\)PO\(_4\), matching the concentration of \(^{31}\)P in the human muscle [24]; 10 g/L methacrylic acid to reduce convection; and 1 ml/L Gd-based contrast agent to reduce \(T_1\). The dielectric properties were measured using a custom-built probe [127] and a network analyzer (E5061B; Agilent, Santa Clara, CA, USA). At the frequencies of interest, i.e., 120.3 and 297.2 MHz, the determined values of relative permittivity were \(\varepsilon_r = 80.1\) and 75, and the specific conductivities were \(\sigma = 0.36\) and 0.59 S/m, respectively.

Coil Design

As a starting point for the design of the new coil, the number of elements for \(^{31}\)P and \(^1\)H were set to three and two, respectively. All five coil elements were driven as transceivers, allowing for static \(B_0^+\) shimming.

A custom-built coil interface was constructed containing a three-way Wilkinson power divider for \(^{31}\)P and a 90° hybrid coupler for \(^1\)H, as well as one transmit/receive switch and preamplifier for each channel, as illustrated in Figure 1b. Considering applications in the Gm and Sol muscles, the coil was shaped in the form of a half cylinder, providing close form-fitting of the coil elements to the posterior part of the human calf. In this configuration, the calf is kept close to its natural shape, even when moving during exercise. The coil housing is made of acrylic glass and has an inner diameter of 14 cm (Fig. 4.1c).

The width of the coil elements was chosen to cover the half cylinder and provide a sensitive area of about 10 cm in length along the leg. This resulted in three rectangular elements of 6.4 \(\times\) 10 cm\(^2\) for \(^{31}\)P, and two quadratic elements of 12.5 \(\times\) 12.5 cm\(^2\) for \(^1\)H, bent to a diameter of 14.9 and 16.9 cm for the \(^{31}\)P array and the \(^1\)H array, respectively (Figs. 4.1a,b).

For both arrays, copper wires with a diameter of 1.5 mm were evenly split to segments.
4.3. Methods

Figure 4.1: Coil geometry and interface box. (a) Cross-section of the form-fitted coil array with the two $^1$H channels (blue) and the three $^{31}$P channels (red). The light blue area represents a leg phantom (diameter = 14 cm, length = 20 cm). (b) In the top view of the array, the arrangement of the coil elements and their respective connections to the interface box via matching networks (M) and coaxial cables with corresponding cable traps (CT) are illustrated. The interface box, shaded in gray, contains a 90°-hybrid coupler for the $^1$H transmit signal and a three-way Wilkinson power divider for the $^{31}$P transmit signal, as well as transmit/receive switches (T/R) and preamplifiers (triangles) for each channel. (c) A photograph of the coil array in its acrylic glass housing and two $^1$H -cables plus three $^{31}$P -cables, respectively.

of length $< \lambda/20$ by inserting capacitors. The coil elements were tuned to the respective Larmor frequencies, that is, 120.3 MHz for $^{31}$P and 297.2 MHz for $^1$H, respectively, using fixed and variable capacitors (Temex Ceramics, Pessac, France). The coils were matched to 50 $\Omega$ while loaded by a human calf.

To block common mode currents, five floating cable traps [57] were placed on the feed cables. Three traps, tuned to the proton frequency, were located inside the coil housing; another proton frequency trap and a phosphorus frequency trap were placed over all five coaxial cables outside the housing. The design of the coil was investigated employing 3D electromagnetic simulation, comprising interelement decoupling [42, 115, 46, 121] and optimization of static $B_1^+$ shimming [128, 129]. Details of the simulation procedure are described in the following section. The best-performing design, using shared capacitors
on common conductors between array elements, was built. To obtain an optimized static $\mathbf{B}_1^+$ shim, the elements were connected to the coil interface with cables of different lengths, corresponding to the phase delay derived from the simulations.

**Electromagnetic Field Simulations**

Because different calf anatomies may introduce very different loading conditions for the coil, it was of prominent interest to achieve an array design providing high robustness in performance for various loads using a fixed set of capacitor values and a fixed phase setting.

The chosen $^{31}\text{P}$ array design was then compared to two other RF coil types, a single channel loop coil and a high-pass birdcage coil, all of equal radius (see below).

The simulations used in this work were based on a combination of full-wave 3D electromagnetic simulation and RF circuit cosimulation [64], performed using commercial software (XFtdt 7.3; Remcom, State College, PA and ADS; Agilent, Santa Clara, CA). Because the investigated coil is a local transmit coil, local RF power deposition had to be estimated to meet the regulations of the International Electrotechnical Commission (IEC) guideline 60601-2-33 [37]. Postprocessing for RF coil performance and local specific absorption rate (SAR) evaluation was done using a dedicated toolbox (SimOpTx; Research Studio Austria, MedUni Vienna, Austria) employing local power correlation matrices [65, 66] computed by an ultrafast convolution-based SAR averaging algorithm [130].

For additional safety evaluation, a Pennes bioheat simulation was conducted on all four individual voxel models following the approach of Collins et al. [131], where the coil array was driven with the maximum permissible power that is limited by the local 10 g averaged SAR. The material properties of the tissue types used in the individual voxel models were defined according to literature [131]. The relevant constants for muscle tissue were density $\rho = 1050$ kg/m$^3$, perfusion coefficient $w = 5$ mL/100 g/min, heat capacity $c = 3500$ J/kg/K, thermal conductivity $k = 0.5$ W/m/K, and metabolically generated heat $Q_m = 750$ W/m$^3$. The values for fat tissue were set to $\rho = 943$ kg/m$^3$, $w = 2.8$ mL/100 g/min, $c = 2300$ J/kg/K, $k = 0.25$ W/m/K, and $Q_m = 300$ W/m$^3$.

**Individual Voxel Models**

To optimize coil performance at high-resonance frequencies by simulation in a realistic usage scenario, suitable 3D models of different human calves were employed. Individual models for four healthy subjects (Fig. 4.2a) were generated from high-resolution water- or fat-saturated images of the volunteers’ calves using the $^1\text{H}$ channels of the presented calf coil. The images were segmented into compartments of muscle with high permittivity ($\varepsilon_r \approx 68$) and conductivity ($\sigma \approx 0.73$ S/m) and fat with low permittivity ($\varepsilon_r \approx 13$) and
conductivity ($\sigma \approx 0.07 \text{ S/m}$), using MATLAB R2012b (MathWorks Inc., Natick, MA, USA)—providing sufficient accuracy for prediction of RF power deposition in the human extremities [132]. Acquiring these data using the same coil has the advantage of shaping the calf to the coil housing, which enables exact positioning of the voxel model data in the 3D EM simulation.

Figure 4.2: Individual voxel models and simulated $^{31}\text{P} \mathbf{B}_1^+$ fields. (a) The voxel models (female (fem) 1, fem 2, male 1 and male 2) derived from $^1\text{H}$ images acquired with the proton part of the proposed array coil are representative of different calf types with regard to gender-specific differences in fat layer thickness and training-related effects of muscle volume. Three regions of interest are marked in each model: a voxel for localized spectroscopy studies in the gastrocnemius medialis muscle (Gm), a voxel in the soleus muscle (Sol), and the lower half cylinder (shaded light blue area). The positions of the phosphorus coil channels are indicated (Ch 1–3). (b) The simulated $\mathbf{B}_1^+$ distribution for the final coil design with shared conductors and a globally optimized phase combination for $\mathbf{B}_1^+$ shimming is shown for the four individual voxel models.

Decoupling Schemes

To provide a good choice for the decoupling scheme of the $^{31}\text{P}$ coil elements, three different array designs were investigated (Fig. 3). Conventional overlap decoupling (OL) [42, 133, 134], a shared conductor (SC) design with decoupling capacitors [119, 135, 136], and an overlap design combined with a shared capacitor between the outer two elements (OL+SC) were compared using the four voxel models described above for each decoupling scheme.

Tuning, matching, adjustment for the decoupling capacitors, as well as scaling parameters (45), were obtained using circuit cosimulation. The best overlap for the OL and OL+SC designs was determined by 3D simulation of both arrays—with varying overlap from $7^\circ$ (9.6 mm) to $10^\circ$ (13.7 mm) — in $0.25^\circ$ (0.34 mm) steps, without readjusting the capacitor values. The best overlap was defined as the configuration for which the average decoupling value and its standard deviation were minimal. For the three array designs, the overall
length and width of the array was kept constant, yielding slightly smaller coil elements for the shared conductor design. The element size was $7 \times 10$ cm$^2$ for the overlapping arrays (OL and OL+SC), whereas for the SC array the element size was $6.4 \times 10$ cm$^2$. B- and E-fields of the individual coil elements were simulated for each voxel model separately.

**B$_1^+$ Shimming**

To obtain the phase settings for B$_1^+$ shimming, three regions of interest (ROIs) were defined in each voxel model (Fig. 4.2a), corresponding to realistic applications. The ROIs selected are the lower half cylinder covered by the coil housing, and two double-oblique cuboid voxels situated in the Gm and Sol muscles, respectively. B$_1^+$ was evaluated in each of these ROIs and using all four voxel models. For each ROI, the relative phase shifts between the channels of both arrays were varied from $-180^\circ$ to $+175^\circ$ in steps of $5^\circ$, one channel being fixed to a phase of $0^\circ$ without loss of generality. This yielded $5184(=72^2)$ phase combinations for the phosphorus coil array and 72 phase combinations for the proton array. Local power deposition in terms of SAR was determined for each decoupling design in all four voxel models. The combined electromagnetic field in each ROI can be optimized with respect to transmit efficiency $E$,

$$E = \frac{B_1^+}{\sqrt{\text{max}(\text{SAR}_{10g})}}$$

(4.3.1)

where $\text{max}()$ denotes the maximum value; the relative inhomogeneity $I$

$$I = \frac{\text{std}(B_1^+)}{B_1^+}$$

(4.3.2)

where $\text{std}()$ denotes the standard deviation; or a combination of both. In this study, the product $f$ of normalized transmit efficiency and 1-normalized relative inhomogeneity

$$f = \frac{E}{\text{max}(E)} \cdot \left(1 - \frac{I}{\text{max}(I)}\right)$$

(4.3.3)

was used as the target function to be maximized for optimization of the B$_1^+$ shim. This approach accounts for B$_1^+$ homogeneity as well as for B$_1^+$ efficiency.

From this calculation, optimal phase settings were determined for each subject and ROI with respect to the target function. Due to practical reasons, it would be favorable to obtain a single phase setting suitable for a range of different subject anatomies and target ROIs. Obviously, when employing a globally optimized phase combination instead of individually determined optima, a certain decrease in transmit efficiency and/or homogeneity must be accepted. To quantify this effect, and to determine whether a global average can be used, the coil performance using the arithmetic mean of the individually optimized phase combinations over all subjects and ROIs was compared to the performances at the respective subject- and ROI-specific optimum.
The derived maximum 10-g averaged SAR values of both the $^1$H and the $^{31}$P array were used to determine the power safety limits to ensure safe use of the RF coil in vivo.

**Comparison to Other Coil Types**

To compare the performance of the $^{31}$P array to existing RF coil designs, additional simulations of two other coil types were conducted. A single channel form-fitted loop coil with dimensions equal to the overall size of the array ($19.2 \times 10$ cm$^2$, bending diameter $14.9$ cm) and a similarly sized quadrature-driven 16-leg high-pass birdcage (length $= 10$ cm, diameter $= 14.9$ cm) were modeled within XFtdt (Remcom) (see schematics at the top of Figure 4.5). The coils were loaded with a 20-cm-long quasi-cylindrical phantom with flattened top (diameter $= 14$ cm), comparable in cross-section to a normal human lower leg. Its dielectric properties were set to $\varepsilon_r = 50$ and $\Sigma = 0.25$ S/m. The postprocessing procedure described in the previous paragraphs was used to evaluate the coil performances. For a valid comparison, the appropriate safety limits [37] for volume and surface coils were considered, and all three coils were driven with the maximum permissible power. The mean $B_1^+$ and relative inhomogeneity were calculated in each ROI.

For a comparison including receive sensitivity, a figure of merit $\mu$, proportional to SNR [31], was calculated following the approach presented by Lemdiasov et al. [36]. The figure of merit $\mu$ is defined as:

$$\mu^2 = \frac{2[I^*]^T[B_1^*][B_1]^T[I]}{[I][R][I]} \quad (4.3.4)$$

where $B_1$ denotes the vector of the $B_1$ field at a specific point in space for all available RF coil channels, based on the condition that a current of 1 A (ampere) is supplied into the respective channels, whereas the remaining channels are supplied with 0 A (open circuit); the superscript $^T$ denotes the transpose of the according matrix. The vector $I$ comprises weighting factors that are chosen to maximize SNR [42, 31], and the asterisk denotes the complex conjugate. The resistance matrix $R$ was derived from the system’s scattering parameter (S-parameter) matrix when no matching capacitors were present ($S_{\text{no}_m}$).

Depending on the number of channels, this resistance matrix is a scalar (single-loop coil), a $2 \times 2$ (birdcage coil), or a $3 \times 3$ (array coil) matrix:

$$R = \text{Re}(Z) = \text{Re}\left(\frac{I + S_{\text{no}_m}}{I - S_{\text{no}_m}}\right) \quad (4.3.5)$$

where $Z$ denotes the impedance matrix, $Z_0$ is the characteristic impedance of the system ($50$ $\Omega$), and $I$ is the identity matrix. Because the simulation incorporated lossy materials and lumped elements, this resistance matrix represents all present losses, that is, conductors, lumped elements, radiation, and the losses in the sample load. The ratios for $B_1^+$, relative inhomogeneity, and SNR for the array versus the other two designs were calculated and compared, also within the three ROIs (Gm, Sol, and the half cylinder).
Bench Measurements

RF coil characteristics were examined with the network analyzer. Transmission and reflection S-parameters were measured for each subject for all five channels, each at both frequencies. The S-parameter matrix was averaged over the five subjects. The performance of the interface box was measured in terms of transmission losses and input/output isolation of the used T/R switches. Quality factors were determined by the -3 dB bandwidth method from $S_{21}$ measurements with a pair of overlap–decoupled pickup loops for the single array elements [40]. Because the coil is unshielded, the tuning and matching performance was investigated outside and inside the scanner.

Hardware and Setup

A 7 T whole body MRI system (Magnetom 7 T MRI; Siemens Medical, Erlangen, Germany) equipped with an SC72d gradient coil (maximum gradient strength of 70 mT/m and slew rate 200 T/m/s) was used for MR measurements.

MR Measurements

For the individual voxel models, water- and fat-saturated images were acquired using 3D gradient echo $^1$H images with 1-mm isotropic resolution (TR = 20 ms, TE = 2 ms, MA = 256 × 256 × 144) acquired, in 3 min each. For water images, fat suppression was used and vice versa.

To validate the SAR simulations of the $^{31}$P array, and to experimentally assure safe use of the proposed coil array, MRI-induced temperature change was measured and validated qualitatively and quantitatively with the use of fiber optic probes (model T1; Neoptix Inc., Québec, Canada) within the leg phantom. To enable rapid RF-heating, the safety limits determined for this coil were increased. SAR and temperature change follow a linear relationship as long as heat conduction and convection are negligible [137],

$$\text{SAR} = c_{\text{phantom}} \frac{\Delta T}{\Delta t}$$  \hspace{1cm} (4.3.6)

where $c_{\text{phantom}}$ denotes the heat capacity of the phantom, which is approximately equal to the heat capacity of H$_2$O ($\approx 4.2$ J/g/K), and $\Delta t$ is the time period of heating. For calculation of the RF-induced temperature increase, the proton resonance frequency shift (PRF) method [88] was used, in which the temperature-induced phase shift is calculated from phase maps before and after temperature change. To avoid contributions from heat conduction, a preliminary experiment with fiber optic probes was conducted to determine the time period for which the temperature increases linearly with the use of fiber optic probes [137].
The temperature-mapping protocol consisted of three consecutive measurements, starting and concluding with a gradient echo phase map (TR = 85 ms; TE = 80 ms; 1 slice; 5-mm slice thickness; voxel size = 1.2 × 1.2 mm$^2$). In between, a gradient echo-based sequence with short repetition time and high RF power was used to heat the sample. The unaveraged SAR, calculated for the same input power as applied in the temperature-mapping protocol, is then directly proportional to the change in temperature (Eq. 4.3.6). To validate the temperature increase measured by MRI, the fiber optic probe remained in the phantom during all measurements. Its position in the middle of the coil at the bottom of the phantom housing is indicated by an arrow in Figure 7a. To avoid artifacts from the probe, the slice of the temperature map was chosen at 2-cm distance from the probe.

The noise correlation matrix was obtained by measuring a free induction decay sequence without excitation pulse for $^1$H and $^{31}$P.

To demonstrate in vivo applicability of the coil, localized $^{31}$P MR spectra were acquired using a slice selective excitation combined with localization by adiabatic selective refocusing (semi-LASER) sequence [105] with a TR of 6 s. The two volumes of interest (VOI) were located in the Gm (VOI ≈ 42 cm$^3$) and Sol muscles (VOI ≈ 50 cm$^3$). The respective sequence parameters were TE = 24 ms, refocusing pulse duration = 3.4 ms, 5 averages in the Gm muscle; and TE = 29 ms, refocusing pulse duration = 4.6 ms, 5 averages in the Sol muscle. After 2 min of rest, the subject performed 5 min of plantar flexion exercise on an MR-compatible ergometer [138]. This protocol was executed twice, first with the VOI placed in the Gm muscle, then for the Sol muscle, with a 20-min resting period in between to allow the phosphocreatine and inorganic phosphate levels to recover after exercise. Exponential line broadening of 7 Hz and zero filling to 4096 points were used for display. Noise was decorrelated during reconstruction of the $^{31}$P spectra [42].

### 4.4 Results

#### Electromagnetic Field Simulations

**Decoupling Schemes**

The simulation results for the decoupling schemes of the investigated $^{31}$P array are summarized in Figure 3. The classical OL array (blue) exhibited its optimum at an overlap of 7.25°, but shows the least favorable mean interelement decoupling (Fig. 4.3a) among the three investigated designs. The combined overlap and shared capacitor scheme (OL+SC; red) showed very good decoupling between the next-nearest neighbors due to the shared capacitor and slightly improved nearest-neighbor decoupling, compared to the OL array. This is because the overlap between neighboring elements can be optimized without be-
ing limited by the coupling of the next-nearest neighbors, exhibiting its optimum at an overlap of 7.75°. The SC array performed best in terms of the highest mean decoupling between channels and the smallest variance across calf anatomies. The arithmetic mean of the reflection coefficients converged at -20 dB or better for all coil types (Fig. 4.3b) indicating that the elements were well matched to 50 Ω. In terms of transmit efficiency (Fig. 4.3c), negligible differences between the three methods were observed. From Figure 3d, it can be seen that the OL+SC and the SC configurations exhibit considerably better homogeneity than the overlapped array. Based on these findings, the shared conductor array design was chosen for the coil that was built and used in all MR experiments.

**Figure 4.3:** Performance comparison of different decoupling schemes for the $^{31}$P array. Overlap decoupling (blue, left), overlap with shared capacitor (red, center), and shared conductor decoupling (green, right) have been compared. The geometric arrangements of the three designs are illustrated in the top row. The S-parameters for each design are displayed in two subfigures: (a) inter-element decoupling and (b) element matching to 50 Ω. The bottom row depicts (c) transmit efficiency and (d) relative inhomogeneity. Error bars represent the average absolute deviation across the four investigated voxel models. The shared conductor design shows the best inter-element decoupling. Together with the overlap decoupling + shared capacitor approach, it provides better homogeneity within the half cylinder ROI defined in Figure 4.2a, compared to the classical overlap. Negligible difference in transmit efficiency was found.
4.4. Results

Figure 4.4: \( B_1^+ \) shimming of the three element \(^{31}\text{P} \) array. Data for the half cylinder ROI in the female subject 1 is shown as an example. For the other subjects and ROIs, analogous data has been obtained. Values for (a) transmit efficiency, (b) relative inhomogeneity, and (c) the optimization target function, are plotted as a function of transmit phase offsets of coil channels 2 and 3 (\( \varphi_2 \) and \( \varphi_3 \)), respectively. The corresponding optimized phase-offset values are overlaid and marked with a white arrow in the image to the right. *a.u., arbitrary units.

\( B_1^+ \) Shimming

Figure 4.4 shows \(^{31}\text{P} \) transmit efficiency \( E \) (Fig. 4.4a), relative inhomogeneity \( I \) (Fig. 4.4b), and the target function \( f \) (Fig. 4.4c) for one exemplary dataset (half cylinder ROI; female 1). The phase combination scoring highest with respect to the target function was considered the subject-specific and ROI-specific optimum, highlighted by a white arrow. The globally optimized phase combination, obtained by averaging over all subject-specific and ROI-specific optima, was found to be 0°, −66 ± 8°, and −129 ± 3° for channels 1, 2, and 3, respectively. The spatial distributions of simulated \(^{31}\text{P} \) transmit fields using the globally optimized phase combinations are displayed in Figure 4.2b for all four subjects. The effects on transmit efficiency and homogeneity, when using the globally optimized phase combination instead of the individual optima, are summarized in Table 4.1. For \(^{31}\text{P} \), an acceptable average transmit efficiency degradation was determined to be 2.4% ± 1.8. Only very subtle changes of < 1.6 percentage points (pp) in relative inhomogeneity were observed. Because there are only two \(^1\text{H} \) array elements, there is only one free phase parameter. The optimized average phase offset between the two channels was found to be 90 ± 7°. Also for the \(^1\text{H} \) array, only marginal changes in coil performance were observed when using the averaged phase combination optimum; a maximum deviation in transmit efficiency of 4.8% is seen in the female 1, whereas the other subjects showed hardly any changes.

With the derived optimal phase setting, the maximum 10 g-averaged SAR normalized
to the input power $\max(SAR_{10g})/P_{in}$ averaged over all four subjects, was determined as $1.28 \pm 0.04 \text{ kg}^{-1}$ for the $^1\text{H}$ array and $1.59 \pm 0.17 \text{ kg}^{-1}$ for the $^{31}\text{P}$ part. For in vivo experiments, a safety margin of 25% was added to the maximum value.

### Comparison of Different Coil Types

The maximum allowed power for the quadrature-driven birdcage coil, being limited by the partial body SAR guidelines, was calculated to be in the range of 19.0 to 19.2 W, depending on the total body mass (70–90 kg). For the coil array, being additionally limited by local SAR constraints, the maximum permissible power within the normal-operation-mode local SAR limit of 20 W/kg for extremities was 12.2 W; the limit for the single loop was 10.7 W. Mean $B_1^+$, relative inhomogeneity, and mean 1 for the three ROIs and coil types are summarized in Table 4.2. Higher $B_1^+$ values in the array were observed for all three ROIs in comparison with the other coils. The proposed 3-channel array produces an 85% to 117% higher $B_1^+$ field than the single loop coil, and it outperforms the 16-leg high-pass birdcage by 14% to 31% in the chosen ROIs (Gm, Sol, half cylinder). Due to its higher receive sensitivity, in addition to the higher $B_1^+$, a minimum two-fold increase in SNR (Sol/birdcage) up to 3.2-fold (Gm/single loop) was calculated for the array design. Figure 4.5 depicts the results as $B_1^+$ (Figs. 4.5a,b) and SNR (Figs. 4.5c,d) ratio maps; the top row displays the geometry of the coil models used. The proposed three-channel coil array performs better in the red areas below isocontour 1 (i.e., where performance is

Table 4.1: The changes in transmit efficiency (in %) and relative inhomogeneity (in percentage points, pp) when using the phase combination optimum averaged over subjects and ROIs, instead of the respective subject-specific optima, are summarized for all subjects and ROIs. For the $^{31}\text{P}$ array, negligible performance loss in terms of transmit efficiency is obtained for the female 2 and male 1 subjects, whereas the female 1 and male 2 subjects show slightly higher but still acceptable values below 6%. Only very subtle changes in relative inhomogeneity are observed. Similarly, for the $^1\text{H}$ array, coil performance in the half cylinder ROI is only marginally altered when using the averaged phase combination optimum. *Gm, Gastrocnemius medialis; Hcyl, half cylinder; Sol, Soleus.

![Table 4.1](image-url)
Table 4.2: The mean B$_{1}^+$, relative inhomogeneity, and mean µ-values in the three ROIs, gastrocnemius medialis (Gm), soleus muscle (Sol), and lower half cylinder, show a superior performance of the 3-channel coil array in terms of transmitted B$_{1}^+$ and a figure of merit µ, which is proportional to SNR. The maximal permissible power according to IEC60601-2-33 was used, enabling a valid and realistic comparison of the surface coils and the volume coil. *Gm, Gastrocnemius medialis; Hcyl, half cylinder; Sol, Soleus; a.u., arbitrary units.

4.4. Results

Bench Measurements

The coil was sufficiently matched for all four volunteers with an arithmetic mean of reflection coefficients $<-26$ dB for the $^1$H array and $<-17$ dB for the $^{31}$P array, respectively. Sufficient interelement decoupling was achieved for both the $^{31}$P array ($<-12$ dB) and the $^1$H array ($<-23$ dB). The full S-parameter matrices are shown in Figure 4.6. The Q-ratio ($Q_{\text{unloaded}}/Q_{\text{loaded}}$) for single $^{31}$P elements was $\approx 8$, and $\approx 10$ for $^1$H elements, showing strong sample loss dominance. The observed crosstalk between $^1$H and $^{31}$P arrays was $<-16$ dB at 120.3 MHz and $<-35$ dB at 297.2 MHz. The input–output isolation for the $^{31}$P/$^1$H T/R switches in the interface box that were used to connect the coil to the scanner were $<-36.7$/$-40.5$ dB, respectively. The overall transmission losses, including T/R switches, Wilkinson power divider ($^{31}$P), and 90° hybrid coupler ($^1$H), were determined as $-3.6$ dB for the $^{31}$P and $-2.6$ dB for the $^1$H transmit path. No considerable alterations in tuning and matching were observed when introducing the coil into the scanner bore.
Figure 4.5: Comparison of the 3-channel $^{31}$P array, with an equally sized single-loop coil and a quadrature 16-leg high-pass birdcage. The geometries of the simulated coils are shown in the top row. Ratio maps and isocontours of (a, b) the $B_1^+$ field and (c, d) SNR distributions calculated as the ratio of the array’s and the single loop’s (ratio array/single loop) or birdcage coil’s (ratio array/birdcage) values, respectively. In the lower half cylinder, the array outperforms both other coil types with respect to SNR.
4.4. Results

Figure 4.6: Coupling matrices. The coupling matrices including both arrays at both frequencies of interest, that is, 120.3 MHz and 297.2 MHz, are shown. The data were averaged over the four volunteers' calves to incorporate different loading conditions.

MR Measurements

The experiment using fiber optic probes showed a linear temperature increase for 110 s, before the curve started to flatten, indicating that heat conduction began to influence the temperature distribution. To ensure the proportionality of SAR and the measured temperature maps, this time period was used for further experiments. In the main heating experiment, the temperature difference (ΔT) measured with the fiber optic probe was 0.33°C, closely matching the calculated value of 0.29°C. Figure 4.7a shows the measured temperature distribution as obtained with the PRF method [88]. Figure 4.7b shows the simulated unaveraged SAR distribution, taking into account the pulse shape, duty cycle, and input power of the employed heating sequence—including the measured losses along the RF chain and the Q-factors of the $^{31}$P array. The dissipated power was estimated to be 16.3 W. The measured and simulated temperature/SAR distributions match well, both qualitatively and quantitatively, validating the numerical methods used for the safety-relevant SAR simulations. A pixel-wise linear regression showed a 13% overestimation of temperature increase by simulation with an $R^2$ of 0.88. Note that this unaveraged SAR distribution for calculation of the temperature increase is not the 10 g average used for determination of the safety limits.

Noise correlation was measured to be below 15.8% and 27.8% for the $^1$H and $^{31}$P array, respectively.

Four spectra of a single subject, acquired at rest and after 5 min of exercise in the Gm and Sol muscles, are displayed in Figure 4.8. As a consequence of different muscle recruitment, a 94% decrease of PCr signal was observed in the Gm muscle, whereas the PCr decrease was only 23% in the Sol muscle, with the same exercise intensity. The shift of the Pi peak toward the PCr resonance indicates acidification (pH = 6.6) in the Gm muscle, whereas the pH in the Sol muscle was alkaline during exercise and returned to 7.05 toward the end of exercise.
Figure 4.7: Proton resonance frequency shift and Pennes bioheat simulation temperature and SAR maps. (a) The measured temperature map using the proton resonance frequency method and (b) simulated unaveraged local SAR distribution, both with a dissipated power of 16.3 W, are shown. In case of linear temperature increase, those maps are proportional (see Eq. 4.3.6). The arrow in (a) indicates the position of the fiber optic probe. The images were cropped to exclude areas with strong susceptibility artifacts due to an air bubble. (c) The initial temperature distribution, that is, the physiological starting state, inside a realistic human voxel model of the calf (subject shown: female 1) was simulated using the Pennes bioheat equation. (d) In the steady state condition with RF heating, it can be seen that the maximum allowed temperature of 39°C given by the IEC guideline 60601-2-33 is not exceeded.
4.5. Discussion

Figure 4.8: Localized $^{31}$P MR spectra from the exercising human gastrocnemius medialis and the soleus muscle. (a) Typical position of the voxels placed in the gastrocnemius medialis (Gm) and the soleus (Sol) muscles, overlaid on a $T_2$-weighted proton image obtained with the 2-channel $^1$H-array. (b-e) Spectra acquired every 6 seconds, 5 averages each, from a volume of 42 cm$^3$ (Gm; b, d) and 50 cm$^3$ (Sol; d, e). The setup included an MR-compatible ergometer to acquire spectra during rest (2 min) and exercise (5 min) with the proposed RF coil. The spectra in (b, c) were acquired during the period of rest, spectra in (d, e) after 5 min of plantar flexion exercise. Spectra were apodized (7 Hz exponential filter) and zero-filled ($2^x$) for display. Different levels of changes in PCr and pH were observed depending on the muscle (i.e., Gm and Sol muscles), indicating different levels of participation in the exercise task.

4.5 Discussion

A three-channel $^{31}$P, 2-channel $^1$H transceive coil with fixed tuning and $B_1^+$ shimming was designed, simulated, and built. The chosen design for the $^{31}$P array with three channels in a half cylinder arrangement has been shown to increase sensitivity for studies in the Gm and Sol muscles compared to a single channel coil, while restricting complexity in postprocessing of spectroscopic data and coil element decoupling compared to an even higher number of channels [139].

Improved coil performance in its application scenario, compared to other coil designs with equivalent parameters, was demonstrated in simulation. Compared to an equally sized and form-fitted single loop coil, an increase of $B_1^+$ by a factor of 2 and of SNR by a factor of up to 3 can be achieved for the Gm and Sol muscles, respectively. An advantage of 30% in mean $B_1^+$ and a factor of up to 2.6 in mean SNR can be obtained versus a similarly sized birdcage coil for these ROIs. This indicates that most of the improvement with respect to the birdcage coil comes from the receive sensitivity of the array, but also a slight improvement in terms of transmit efficiency; thus, $B_1^+$ per applied voltage was to be gained. As expected, both the simulated transmit and the receive fields of the birdcage coil were more homogeneous. For single voxel spectroscopy, however, a spatially broad homogeneity is of less importance, depending on size and position of the volume of interest. This can be seen in Table 2, where the inhomogeneity in the Sol muscle voxel
for the 3-channel array is even smaller than for the birdcage coil. Also, to alleviate the inherent inhomogeneity of surface coils, adiabatic excitation pulses can be employed to obtain a homogeneous excitation \cite{140, 141}. The simulated higher transmit efficiency for the proposed array facilitates the use of such pulses because the adiabatic condition can be more easily fulfilled.

EM simulations performed using individually generated voxel models of different calf anatomies of healthy volunteers within a normal BMI range show good performance stability of the coil with anatomic variability. These simulation results and the experimental findings justify our approach for fixed tuning, matching, and \( B_1^+ \) shimming. In addition, bioheat simulations provide evidence that legal temperature limits are not exceeded, even after about 90 min of full RF excitation, which is well beyond any practical protocol used.

In-vivo applicability was successfully demonstrated in a localized \( ^{31}P \) MRS experiment in exercising, normal human calf muscle. The spectral quality permits the quantification of metabolic differences between the two neighboring muscles, namely, Gm and Sol. The exemplary data set shows metabolically different reactions to plantar flexion exercise in these two distinct muscles. A more detailed analysis of exercise physiology, however, is beyond the scope of this technical paper. In other reports, initial results of dynamic \( ^1H \) and \( ^{31}P \) studies of the exercising calf muscle using the presented coil array have been demonstrated \cite{102, 104, 108}, revealing a two-fold PCr–SNR increase over a commercially available standard planar 10-cm loop coil in the Gm muscle \cite{108} in a single voxel \( ^{31}P \) MR measurement.

In future work, crosstalk between \( ^{31}P \) and \( ^1H \) channels could be further reduced by inserting second order traps \cite{118, 142} into the \( ^{31}P \) channels. For studies in which the more ventral muscles of the calf are of interest, extended coverage of the coil to the tibialis and peroneus muscles would be needed. In view of metabolic studies on diabetic patients, future investigations should also include subjects with higher BMI.

4.6 Conclusion

In conclusion, simulations show that the presented 7 T multinuclear RF coil array provides higher transmit efficiency and SNR than a comparably sized single-loop or birdcage coil in ROIs for \( ^{31}P \) metabolic studies of the calf muscles. Together with the higher magnetization available at 7 T, this improves data quality in single-shot localized spectroscopy.
There were three main studies conducted with the proposed RF coil, all of which were concerned with gaining insight into calf muscle metabolism when performing plantar flexion. A detailed description of each study can be found in the cited publications.

**Study 1** was designed to quantify the degree of recruitment of two different muscles, namely the gastrocnemius medialis and the soleus muscle (see Fig. 5.1b), with the help of single voxel spectroscopy. It was published under the title "Localized semi-LASER dynamic \(^{31}\)P magnetic resonance spectroscopy of the soleus during and following exercise at 7 T" in "Magnetic Resonance Materials in Physics, Biology and Medicine", 2015 [143].

**Study 2** was designed to quantify the perfusion of the calf muscles noninvasively during exercise with the help of pulsed arterial spin labeling. The work entitled "Dynamic ASL and \(T_2^*\)-weighted MRI in exercising calf muscle at 7 T: A feasibility study" was published in "Magnetic Resonance in Medicine", 2014 [126].

**Study 3** was designed to establish direct relationships between \(T_2\) changes, pH kinetics, and PCr dynamics in exercising calf muscles, again with the help of single voxel spectroscopy. The work was published in "NMR in Biomedicine" under the title "Exercising calf muscle \(T_2^*\) changes correlate with pH, PCr recovery and maximum oxidative phosphorylation", 2014 [125].

The setup for each study included a nonmagnetic, pneumatic ergometer (designed and built in-house by Dr. Martin Meyerspeer) constructed to fit in the scanner bore to realize plantar flexion with adjustable, constant force. The developed RF coil was used on the right lower leg. The measurement protocol consisted of 2 min at rest for baseline measurements, 5 min of plantar flexion followed by either 7 min or 20 min recovery for spectroscopy and imaging sequences, respectively. The setup including the coil and the ergometer can be seen in Fig. 5.1a. The muscles of interest are shown overlayed on a 2D
GRE image acquired with the proposed RF coil in Fig. 5.1b. During the 5 min of exercise the volunteers were asked to perform two pedal pushes after each imaging/spectroscopic acquisition (TR=6 s).

(a) Measurement setup consisting of the non-magnetic ergometer (yellow) and the developed $^1$H/$^{31}$P RF coil (green)

(b) Muscles of interest, gastrocnemius lateralis (red), medialis (green), and soleus (yellow)

Figure 5.1: The measurement setup for the conducted studies is showed in (a). The muscles of interest for the investigations are shown in (b).

The exact imaging parameters can be found in the respective publication, and are stated in as shortened version in Tab. 5.1. Study 1 executed two equivalent measurement bouts, spaced 30 min apart, with the difference being the position of the acquisition voxel (once in GM, once in SOL).

<table>
<thead>
<tr>
<th>Protocol</th>
<th>Sequences</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 min rest</td>
<td>semi-LASER single voxel spectroscopy</td>
</tr>
<tr>
<td>5 min exercise</td>
<td>single shot (TR=6 s), TE=24 ms (GM), 29 ms (SOL), 5 averages</td>
</tr>
<tr>
<td>7 min recovery</td>
<td>Refocusing pulse duration=3.4 ms (GM), 4.6 ms (SOL)</td>
</tr>
<tr>
<td>2 min baseline</td>
<td>Multi echo GRE for $T_2$ and positioning: TE=4.5 ms, 9 ms, and 14.5 ms</td>
</tr>
<tr>
<td>5 min exercise</td>
<td>pulsed ASL with FAIR labeling, SQ2TIPS, and single slice EPI readout, MA 128x128, FOV 160x160x6 mm³</td>
</tr>
<tr>
<td>20 min recovery</td>
<td>sampling scheme: 6/8 partial phase encoding (PPE) + GRAPPA 2 (TE=20 ms), Q2TIPS = 200 ms</td>
</tr>
<tr>
<td>2 min baseline</td>
<td>Anatomical reference: axial GRE (30 slices, FOV= 160x160x4.8 mm, MA= 256 x 256, TE=4.5 ms, TR = 570 ms</td>
</tr>
<tr>
<td>5 min exercise</td>
<td>EPI: TR=6 s, TE = 20 ms, 270 repetitions, slice thickness 6 mm, MA 128x128</td>
</tr>
<tr>
<td>7 min/20 min recovery</td>
<td>semi-LASER (GM): TR=6s, TE=24 ms</td>
</tr>
</tbody>
</table>

Table 5.1: Protocol and sequence parameters for the three conducted studies.

Study 1 has included 11 healthy volunteers, 16 healthy volunteers participated in study 2, and 19 healthy participants were investigated in study 3. Written, informed consent was obtained from all subjects in agreement with local ethics regulation and according to the latest version of the Declaration of Helsinki.
5.1 Results and Conclusions

**Study 1** showed different recruitment degrees for gastrocnemius medialis and soleus muscle when using plantar flexion (with straight knee) in terms of PCr kinetics. In Fig. 5.2a the stackplot of single shot (TR=6 s) spectra without averaging in the gastrocnemius medialis and soleus muscle during rest, exercise, and recovery can be seen. Fig. 5.2b shows the time series signal of PCr and Pi in both muscles of interest. It clearly can be seen that in case of plantar flexion with straightened knee, the GM is the main muscle that is recruited for this exercise, yielding an average depletion of 94% PCr. The soleus muscle does contribute to the muscle workload necessary, but only in a very minor fraction.

![Stackplot of single shot spectra in GM and SOL](image)

(a) Stackplot of single shot spectra in GM and SOL

(b) Timeseries of PCr and Pi signal in SOL(a) and GM(b)

**Figure 5.2:** Results from study 1 as published in [104].

**Study 2** showed the feasibility of measuring perfusion in the exercising calf muscle using arterial spin labeling (ASL) on 7 T. Fig. 5.3a depicts a post exercise perfusion map, showing increased values mainly in the gastrocnemius medialis and lateralis, which is consistent with the results of study 1. Fig. 5.3b shows the relative signal change of pre

![Perfusion map and EPI](image)

(a) Perfusion map

(b) EPI

**Figure 5.3:** Results from study 2 as published in [126].
exercise value and post exercise maximum, overlayed on a GRE image, again backing up the findings that gastrocnemius bears the main workload.

**Study 3** determined the following correlations between phosphocreatin (PCr), pH and $T_2^*$ time courses. The following table shows the significant Pearson correlations found in the study of 19 healthy subjects: where $\tau_{\text{PCr, rec}}/\tau_{\text{Pi, rec}}$ are the recovery time constants for PCr and Pi respectively, $V_{\text{PCr}}$ is the initial PCr recovery rate, $Q_{\text{max, lin}}/Q_{\text{max, ADP}}$ is the maximum oxidative phosphorylation according to the linear model and ADP-driven model respectively, $\text{pH}_{\text{end, ex}}$ denotes the end exercise pH value, $\text{TTP } S_{\text{EPI}}$ is the post exercise time-to-peak for the EPI signal, and $\Delta S_{\text{EPI}}$ is the magnitude of the post exercise $T_2^*$ change. In conclusion, the study showed a strong connection between skeletal muscle metabolic activity and tissue $T_2^*$ changes.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\tau_{\text{PCr, rec}}$</th>
<th>$\tau_{\text{Pi, rec}}$</th>
<th>$V_{\text{PCr}}$</th>
<th>$Q_{\text{max, lin}}$</th>
<th>$Q_{\text{max, ADP}}$</th>
<th>ADP</th>
<th>$\text{pH}_{\text{end, ex}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCr depletion</td>
<td>$&lt; 10^{-7}$</td>
<td>$&lt; 0.02$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\text{TTP } S_{\text{EPI}}$</td>
<td>$&lt; 10^{-6}$</td>
<td>$&lt; 10^{-6}$</td>
<td>$&lt; 10^{-4}$</td>
<td>$&lt; 0.001$</td>
<td>$&lt; 10^{-4}$</td>
<td>$&lt; 0.001$</td>
<td>$&lt; 0.01$</td>
</tr>
<tr>
<td>$\Delta S_{\text{EPI}}$</td>
<td>$&lt; 0.05$</td>
<td>$&lt; 0.01$</td>
<td>$&lt; 0.01$</td>
<td>$&lt; 0.01$</td>
<td>$&lt; 0.01$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table 5.2:** Pearson correlation p-values for the investigated parameters (if existing), as published in [125].

for PCr and Pi respectively, $V_{\text{PCr}}$ is the initial PCr recovery rate, $Q_{\text{max, lin}}/Q_{\text{max, ADP}}$ is the maximum oxidative phosphorylation according to the linear model and ADP-driven model respectively, $\text{pH}_{\text{end, ex}}$ denotes the end exercise pH value, $\text{TTP } S_{\text{EPI}}$ is the post exercise time-to-peak for the EPI signal, and $\Delta S_{\text{EPI}}$ is the magnitude of the post exercise $T_2^*$ change. In conclusion, the study showed a strong connection between skeletal muscle metabolic activity and tissue $T_2^*$ changes.

**Summary**

All three studies have been possible only through the use of UHF-MR ($\geq 7$ T), a dedicated RF coil applicable for $^{31}\text{P}$ and $^1\text{H}$ nuclei fitting the human calf muscle, optimized imaging and localized spectroscopy protocols. This required a team of scientists and engineers to successfully overcome all the challenges and obstacles that occur along the way.
6.1 Purpose

Phosphorous spectroscopy in the occipital lobe may be used to investigate the $^{31}$P metabolism in the visual cortex and its changes during various conditions. Due to the inherently low relative sensitivity of $^{31}$P and its low abundance in the brain, the hardware for the application has to be optimized for increased detection sensitivity. Increasing the field strength to 7 T already results in higher sensitivity, increased spectral resolution and shorter $T_1$-relaxation times [97] for $^{31}$P spectroscopy in general [95]. Employing RF surface coil arrays further increases the achievable SNR, enabling increase in temporal and/or spatial resolution. Here, a dedicated 3 channel $^{31}$P array combined with a 2 channel $^1$H array conformed to the back of the head for $^{31}$P NMR studies in the human occipital lobe is presented together with preliminary results achieved with the proposed setup.

6.2 Methods

As a starting point, the outline of both arrays was stipulated to be elliptical, with a minor-to-major axis ratio of 0.9. This geometry conforms the human occiput well, since the human head is not a perfect sphere. The proton coil consists of 2 channels sharing the middle conductor and capacitor for decoupling. The phosphorous coil consists of three channels arranged like a "Mercedes"-star. Each element shares a conductor and capacitor with the two neighboring channels, allowing capacitive decoupling between all elements. A schematic of the RF coil can be seen in Fig. 6.1.
6. Development of $^{31}P/^{1}H$ RF Coil for $^{31}P$ Spectroscopy in the Human Visual Cortex

**Figure 6.1:** Schematic of the occipital cortex coil. The blue part depicts the $^{1}H$ array which is hovering above the $^{31}P$ array depicted in red. For channel decoupling the shared conductor and capacitor method is used. The yellow area depicts the occipital lobe where the visual cortex is located, which is the region of interest for the future application. The three body planes, transversal, sagittal and coronal, are additionally plotted and can be used for better visualization of the position of the slices shown in the results section.

### 6.2.1 Numerical Simulation

As outlined in the workflow chapter (ch. 3), the RF coil was simulated ($^{1}H$ and $^{31}P$ array) and optimized ($^{31}P$ only) by FDTD 3D electromagnetic simulation (XFdtd 7.4, Remcom, State College, PA, USA) together with a circuit co-simulation (ADS, Agilent, Santa Clara, USA), and an in-house developed post-processing software package (SimOpTx, RSA, MedUni Vienna, Austria) for SAR evaluation [130].

**Coil dimension and $B_{1}^{+}$ shimming**

To find the optimal coil size in terms of SAR efficiency ($\frac{B_{1}^{+}}{\sqrt{\max(SAR_{10g})}}$) for the $^{31}P$ array, the major axis was varied between 9 cm and 15 cm in four steps. Thereby keeping the distance from the conducting wires to the surface of the head constant, resulting in different coil heights. These four simulations were performed for two head-coil distances, namely 1.5 cm and 2 cm, resulting in a total of 8 setups. For each setup $B_{1}^{-}$, $B_{1}^{+}$, and the 10 g SAR were computed with all possible phase combinations resulting from a 5° phase increment (=5184 possibilities).

The resulting optimal coil size was simulated to incorporate a circumferential copper shielding to reduce radiation losses and cable shield currents. Static $B_{1}^{+}$ shimming for the coil setup was determined in terms of SAR efficiency (SE), transmit efficiency ($\frac{B_{1}^{+}}{\sqrt{P_{abs}}}$, TxE), and relative inhomogeneity (RI) in the ROI and the whole head by 3D EM simulation. Again all 5184 possible phase combinations were simulated and compared to find the optimal combination in terms of those figure of merits (SE, TxE, and RI).
Comparison to Conventional Loop Coil

A performance comparison to a conventional planar loop coil with a diameter of 10 cm was conducted. Maximum permissible power $B_1^+$, as dictated by the maximum 10 g SAR value and the IEC guideline [37], and SNR maps were compared to see what performance could be expected.

6.2.2 Hardware Implementation and MR measurements

The optimized coil design was physically built and evaluated with bench and MRI measurements. The scattering parameters were measured on a network analyzer (E5061B, Agilent, Santa Clara, USA), Q-factors were determined using a double, overlap decoupled pickup loop.

MR measurements were performed on a 7 T MR scanner (Siemens Magnetom, Erlangen, Germany) using the proposed coil. The measurements were performed on a 20 cm spherical phantom filled with a phosphorous containing gel and on a papaya fruit. The $^{31}$P containing gel used is equivalent to the muscle phantoms prepared for the form fitted $^{31}$P/$^1$H calf coil presented in chapter 4. The concentration of $K_2HPO_4$ equals the PCr concentration in skeletal muscle ($\approx 33$ mM). Tuning, matching and decoupling capacitors were kept fixed for all experiments. Images were acquired with a 3D gradient echo sequence for both nuclei. Parameters for $^1$H and $^{31}$P scans were TR/TE=20/5 ms, FOV=160×160×128 mm$^3$, matrix=128×128×30, and TR/TE=80/6 ms, FOV=281×281×281 mm$^3$, matrix=32×32×32, 8 averages, respectively.

6.3 Results

6.3.1 Simulation Results

The highest transmit efficiency could be achieved with a coil setup with the following dimensions: for the $^1$H coil the major/minor axis size was 13 cm/11.7 cm, whereas for the $^{31}$P coil dimensions, major/minor axis size was 11 cm/9.9 cm. The distance from the head surface to the coil wire was set to be 1.5 cm, which yields a coil height of 1.4 cm/1.9 cm for the $^{31}$P and $^1$H array, respectively.

Depending on the region of interest and the figure of merit for optimal performance of the coil the following best suited phase settings were determined (Tab. 6.1). Two regions of interest were defined for the static $B_1^+$ shimming determination. The first ROI was defined as a voxel of size and position comparable to realistic applications, and can be seen in Fig. 6.3 depicted as white boxes. The second ROI was the whole head extending to the shoulders.
Table 6.1: Different phase setting depending on the optimization figure of merit and the respective maximum permissible driving power (MPP) for the two defined regions of interest, a voxel of size and position comparable to realistic applications (ROI 1), and the whole head down to the shoulders (ROI 2).

In addition to the defined figures of merit, the maximum permissible forward power has to be taken into account. This is the maximal forward power allowed without exceeding the legal SAR limits [37]. For a local transmit coil operating in the head region the IEC guideline states that there a limit of 10 W/kg. The $B_1^+$ maps corresponding to the phase settings and maximum permissible driving powers (MPP) stated in Tab. 6.1 are shown in Fig. 6.2.

Comparison to loop coil

The maximum permissible power was determined for both setups. With a maximum 10 g SAR value of 2.82 W/kg obtained with a forward power of 1 W, this yields a maximum permissible power of 3.6 W for the loop coil. In case of the array the maximum 10 g SAR value produced with 1 W input power is 1.47 W/kg (SE optimized phase setup), yielding 6.8 W maximum permissible power. The resulting $B_1^+$ maps can be seen in Fig. 6.3. The comparison of achievable SNR can be also seen in Fig. 6.3. For this purpose, the figure of merit $\mu$ from eq. (4.3.4) was calculated for both coil designs.
6.3. Results

\[ B_1^+ \text{ with } P_{\text{in/max}} \]

**Array**

**Loop**

**optimal SNR**

**Array**

**Loop**

**Figure 6.3:** Sagittal and transversal slices of the \( B_1^+ \) field produced by the array and loop coil when driven with the maximum allowed input power of 6.8 W and 3.6 W, respectively (left). Optimal SNR maps for the array and the loop coil are depicted on the left. The white rectangle depicts the location of a voxel used for single voxel spectroscopy in the visual cortex. The location of the three body planes are depicted in Fig. 6.1

The exact values for the mean \( B_1^+ \) and mean SNR for the array and the loop coil, respectively, in the voxel depicted as a white rectangle in Fig. 6.3 are: Mean \( B_1^+ \): 3.65 \( \mu \)T vs. 2.72 \( \mu \)T for the array and loop, respectively, when driven with 1 W input power. Again taking the maximum permissible power into account yields: 9.51 \( \mu \)T vs. 5.17 \( \mu \)T. This translates to 1.3 and 1.8 times higher \( B_1^+ \) in the ROI, respectively. For SNR the difference is even bigger. In the ROI the mean SNR achieved by the array is 6.99 vs. 3.06 for the loop. This means, a factor of 2.3 higher mean SNR can be anticipated.

6.3.2 Hardware Implementation

The real coil setup can be seen in Fig. 6.4. The elliptical 3 channel \(^{31}\text{P}\) array has major/minor axis dimensions of 11 cm/9.9 cm. The 2 channel \(^1\text{H}\) array for scout imaging has major/minor axis dimensions of 13 cm/11.7 cm. Both arrays were bent to conform to the shape of the human head yielding a coil height of 1.4 cm/1.9 cm for the \(^{31}\text{P}\) and \(^1\text{H}\) array, respectively.

Reflection, transmission, and cross coupling coefficients for the \(^{31}\text{P}\) and \(^1\text{H}\) arrays at both Larmor frequencies (120.3 MHz for \(^{31}\text{P}\), and 297.2 MHz for \(^1\text{H}\)) can be seen in Tab. 6.2.

The Q ratio \((Q_{\text{unloaded}}/Q_{\text{loaded}})\) was 3.1 and 16.2 for the \(^{31}\text{P}\) and \(^1\text{H}\) array, respectively, showing sample noise dominance in both arrays. The optimal phase shift for high SAR
6. Development of $^{31}$P/$^1$H RF Coil for $^{31}$P Spectroscopy in the Human Visual Cortex

Figure 6.4: The figure depicts the built RF coil inside its housing. A copper shield was inserted to reduce radiation losses and cable currents.

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<tr>
<td>Frequency [MHz]</td>
<td>$^{31}$P</td>
<td>$^1$H</td>
</tr>
<tr>
<td></td>
<td>120.3</td>
<td>120.3</td>
</tr>
<tr>
<td></td>
<td>-25.9</td>
<td>-13.5</td>
</tr>
<tr>
<td></td>
<td>&gt;-11.6</td>
<td>&lt;-28.7</td>
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Table 6.2: Full S-parameter set for the RF array measured at both Larmor frequencies, i.e. 120.3 MHz for $^{31}$P and 297.2 MHz for $^1$H at 7 T.

efficiency in the ROI (yellow part in Fig. 6.1) was $[100^\circ/0^\circ/40^\circ]$ for the $^{31}$P channels 1, 2, and 3, respectively, see Tab. 6.1.

6.3.3 MR Measurements

MR measurements were conducted on a papaya and a spherical $^{31}$P phantom (d=20 cm). The results can be seen in Fig. 6.5a, and b. The proton GRE shows good coverage of the whole sample (papaya). The $^{31}$P GRE has inherently lower sensitivity, resulting in a lower resolution. Although a GRE is not a $B_1^+$ map, it gives rough estimation of the possible coverage achievable with the RF probe. The $^{31}$P signal seen in Fig. 6.5b covers approximately the bottom third of the spherical phantom.

Figure 6.5: MR measurements conducted with the proposed RF probe array. (a) shows a gradient echo acquisition of a papaya using the $^1$H part of the proposed design. Good coverage of the whole sample is a promising result. (b) shows a $^{31}$P GRE of a $^{31}$P phantom. The coverage area is comparable to the simulated $B_1^+$ field distribution.
6.4 Discussion & Conclusion

A $^{31}$P/$^1$H coil array was developed to improve $^{31}$P sensitivity in the visual cortex in comparison to a simple 10 cm loop coil. Simulation results show superior performance of the proposed RF coil array not only in terms of transmit performance, but also in SNR gain. The coil was physically built, tuned and matched to the respective Larmor frequencies. For the $^{31}$P coil, solely fixed capacitors were used to increase the voltage stability of the array. The Q-ratios of the two arrays show sample noise dominance.

MR measurements of a papaya and a $^{31}$P phantom show good coverage of the proposed setup and are in good agreement with the simulation results. Since the phantom used for the preliminary experiments contains a higher $^{31}$P concentration ($\approx 33$ mM) than the PCR concentration that can be expected in human brain tissue ($\approx 4$-5.5 mM), the feasibility of measuring in vivo PCR kinetics in the brain will have to be evaluated in future experiments.
7.1 Summary

One goal of this thesis was to devise and implement an efficient workflow for RF coil development. The presented workflow focuses on the development of transmit-receive RF coils. Three-dimensional electromagnetic simulation evolved to be a well-established tool for design optimization and safety evaluation especially in ultra high field MR, and is treated elaborately in this work. The entire workflow is described and illustrated with examples in chapter 3.

In the framework of this thesis, a form fitted phosphorus/proton RF transceive array for 7 T MRS of the human calf was developed (see chapter 4). The main objective of this newly developed coil was high $^{31}$P SNR not only in the vicinity of the surface, but also further into the tissue, to distinguish between neighboring muscle groups, i.e. the gastrocnemius and soleus muscles. A challenge in this type of coil development is the intrinsically low SNR of nuclei other than $^1$H. Therefore it is not easy to predict and evaluate the performance of the X-nuclei part, since common MR visualization methods of the $B_1$ field is not always possible. This is where 3D EM simulation can be especially helpful for design optimization. The inherently high SNR of 7 T together with an SNR increase from the surface coil array showed promising results for $^{31}$P spectroscopy in the exercising skeletal muscle, described in chapter 5. Preliminary results of a $^1$H/$^{31}$P RF coil for $^{31}$P MRS in the human visual cortex are presented in chapter 6.

7.2 Future Work

The workflow presented in this thesis already incorporates elaborate 3D electromagnetic simulation techniques to evaluate RF coil designs during development. The techniques employed herein are also used to calculate the SAR distribution, which is the currently used standard for safety compliance during scanning. Those SAR evaluations and the
subsequently assurance of safety for the patient, get more and more complex with the development of parallel transmit (pTx) systems.

In recent years the MR hardware development was pushed towards higher magnetic field strengths ($\geq 7$ T) to significantly improve the achievable signal-to-noise ratio of the method. Higher fields demand proportionally increased RF frequencies, thus decreasing the wavelength into orders of magnitude similar to or even smaller than the human body regions to be examined. This shortening results in an inhomogeneous distribution of the RF magnetic field due to standing wave effects, severely hampering the diagnostic quality of acquired images.

One approach to tackle this issue involves the mentioned RF excitation scheme called parallel transmission MRI [45, 144]. The main principle of pTx systems is the use of multiple RF coils which are independently driven in terms of time-dependent amplitude and phase (transmit weights), and thus create interfering field patterns to generate an advantageous excitation pattern of choice. One major issue with pTx systems is the highly complex local and global SAR prediction, depending on the wave interference of the individual RF fields transmitted per each channel [65, 145]. In the beginning of pTx, worst-case SAR approaches were employed, where the SAR for any possible combination of transmit weights was calculated [146]. This leads to high overestimation of the actual SAR and, hence, to major unnecessary restrictions for the transmit pulses. Therefore, modern SAR prediction schemes take into account the actual transmit weights used for the examination. The already introduced Q-matrix formalism (see section 2.3.4) enables efficient real-time SAR calculation for pTx systems [65, 66]. The Q-matrix formalism can also be combined with a compression of cells into virtual observation points [147, 148], which reduces the calculation time further, at the cost of an accepted overestimation of SAR due to the cell compression. Recently, a new method was proposed to reduce the computation time of the electromagnetic fields and, therefore, also the SAR computation, to the order of $\approx 4$ min [149, 150]. This reduction ultimately could help to make pTx feasible in clinical practice in the future. The approach uses a combination of a long offline pre-computation phase ($\approx 35-40$ hours) and a very rapid online phase ($\approx 4$ min) where the EM fields are determined. During the slow offline phase, a compressed body-model-specific Green’s function (GF) is calculated. This time consuming calculation has to be done for each body model and frequency independently. The representation of the model, i.e. the GF, is then used in a fast online phase to evaluate the chosen coil design.

In the future, the presented workflow will be extended to incorporate the ability to calculate pTx pulses and the resulting SAR pattern in a reasonable amount of time. Therefore, the proposed ultra-fast EM field evaluation method will be implemented. On the basis of the vast set of model-specific-GFs and a target organ the ideal current pattern [151] in terms of SAR, or SNR can be derived. The knowledge of these current patterns can
Figure 7.1: Enhanced simulation workflow to incorporate the feasibility to rapidly (≈ 5 min) evaluate different coil geometries for different ROIs and voxel models, as well as fast calculation of pTx pulses. The additional simulation workflow steps and methods can be used either for determining the optimal RF coil design for a given ROI during the development phase, or to calculate SAR and pTx pulses shortly before a pTx measurement. The voxel model depiction is by courtesy of the IT’IS Foundation [154].

then be translated in a near-optimal RF coil design for that specific organ, obeying the physical constraints given by the manufacturing process of the application. For the final pTx measurement, the pTx pulses (one waveform for each transmitting element) have to be calculated by solving the transmit SENSE equation [45]. Typical constraints for the solution of the pTx pulses are the resulting SAR and/or hardware limitations such as power amplifier performance. In order to reduce the computation time of the constraint pTx pulse calculation a multi-shift conjugate gradient method will be implemented [152, 153]. A schematic of the planned workflow can be seen in Fig. 7.1

Additionally, the computation of a large database (≈ 300-500) of realistic human body models [155] and their representation as Green’s functions is planned to be incorporated. This database can be used as a basis for investigating the effect of differently sized and shaped humans on the RF coil EM fields, and ultimately the SAR and SNR distribution [156]. Such a database can then also be used for a more precise patient specific SAR evaluation for the pTx pulse calculation. The current state of the art is to use readily available human body models, such as the virtual family/population [70, 155]. As of 2015, the virtual population (IT’IS Foundation, Zurich, Switzerland) has 15 human body models, ranging from an 8 week old girl to a 84 year old man, and 3 pregnant women. It is assumed that the SAR pattern of a similarly shaped real human is equivalent to that of the respective virtual family member. With only one possible match for either man or woman in a certain age range, this can be regarded as far fetched, especially when they are used for pTx safety evaluations. A database of several hundreds of possible matches can help accurately evaluate the patient specific SAR.
The database will also include human models with rife lesions and/or tumors. It is a known fact that tumors, cysts and lesions have altered dielectric properties [157, 158, 159, 160], changing the interaction with EM fields to an unknown degree. Investigating the effect of tumors and such in a large scale has, to my knowledge, not been done before and might be valuable, especially when considering pTx measurements, since SAR hotspots are known to occur at positions where conductive paths for eddy currents are narrow between regions of low conductivity [161].

### 7.3 Conclusion

In conclusion, this thesis presents a comprehensive workflow for RF coil development for UHF applications. Following each devised step yielded the successful construction and validation of a form fitted $^{31}$P/$^1$H transceive array for metabolic investigations of skeletal muscle before, during, and after exercise. High SNR in locations further inside the tissue enables the possibility of single shot, localized $^{31}$P spectroscopy with a time resolution of 6 s, and the ability to distinguish between neighboring muscle groups.
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Conference cost grant for students

Travelcost grant for students

2012 ESMRMB, Student Support Grant.
Conference cost grant for students
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International Peer-Reviewed Journals

Localized semi-LASER dynamic $^{31}$P magnetic resonance spectroscopy of the soleus during and following exercise at 7 T

A novel inductive decoupling technique for flexible transceiver arrays of monolithic transmission line resonators

Dynamic ASL and $T_2^*$-weighted MRI in exercising calf muscle at 7 T - a feasibility study

Power balance and loss mechanism analysis in RF transmit coil arrays

Exercising calf muscle $T_2^*$ time courses correlate with pH, PCr recovery and maximum oxidative phosphorylation

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A 3 channel $^{31}$P and 2 channel $^1$H coil array for $^{31}$P NMR in the visual cortex at 7 T

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Anatomy-specific $B_1^+$ shimming for localized $^{31}$P spectroscopy in the human calf determined by 3D EM simulation


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Relation between PCr recovery from exercise and BOLD response in calf muscle


A multichannel $^1$H/$^{31}$P transmit-receive coil for spectroscopy in the human calf at 7T


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**Talks/Presentations**


**Title**: A 3 channel $^{31}$P and 2 channel $^1$H coil array for $^{31}$P NMR in the visual cortex at 7 T


**Title**: Performance Comparison of a Form Fitted Coil Array Vs. a Quadrature Birdcage Coil for $^{31}$P MRS Studies in the Human Calf at 7T

2013 **Oral Presentation**, Toulouse, France, 30th Meeting of the European Society for Magnetic Resonance in Medicine and Biology.

**Title**: Anatomy-specific $B_1^+$ shimming for localized $^{31}$P spectroscopy in the human calf determined by 3D EM simulation

2013 **Poster Presentation**, Salt Lake City, Utah, USA, 21st Annual Meeting & Exhibition of the International Society for Magnetic Resonance in Medicine.

**Title**: Comparison of decoupling schemes for a three channel $^{31}$P array for the human calf muscle at 7 T using 3D electromagnetic simulation

2012 **Poster Presentation**, Lisbon, Portugal, 29th Meeting of the European Society for Magnetic Resonance in Medicine and Biology.

**Title**: A multichannel $^1$H/$^{31}$P transmit-receive coil for spectroscopy in the human calf at 7T