

Clocking Electrode Design and Phase Analysis for Molecular Quantum-Dot Cellular Automata Based Circuits

by

Faizal Karim

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Abstract

Molecular quantum-dot cellular automaton (QCA) offers an alternative paradigm for computing at the nano-scale. Such QCA circuits require an external clock, which can be generated using a network of submerged electrodes, to synchronize information flow, and provide the required power to drive the computation. In this thesis, the effect of electrode separation and applied potential on the likelihood of different QCA cell states of molecular cells located above and in between two adjacent electrodes is analysed. Using this analysis, estimates of operational ranges are developed for the placement, applied potential, and relative phase between adjacent clocking electrodes to ensure that only those states that are used in the computation, are energetically favourable. Conclusions on the trade-off between cell size and applied clocking potential are drawn and the temperature dependency on the operation of fundamental QCA building blocks is considered. Lastly, the impact of random phase shifts on the underlying clocking network is investigated and a set of universal QCA building blocks is classified into distinct groups based on their sensitivity to these random phase shifts.

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Dedication

This thesis is dedicated to my late father who never let me forget the importance of a good education.

Chapter 1

Introduction

1.1 Motivation

Molecular quantum-dot cellular automaton (QCA) is an emerging nano-scale computing paradigm which utilizes the electrostatic coupling between electronic configurations in neighbouring molecules to perform information processing. This computing paradigm was originally introduced by C. S. Lent [3] and has been extended in recent years to devices based on single molecules [4–6]. Several proof-of-concept QCA devices have been fabricated using silicon-on-insulator (SOI) [7], metallic island implementations operating in the Coulomb blockade regime [8–10], and nano-magnetics [11–14]. A simulation tool exists for this technology [15–18] and has been applied towards the high-level design and exploration of both sequential and combinational circuits [19–21].

A clocking implementation, using a set of submerged electrodes which generate an electric field at the level of the QCA molecules, has been proposed [22]. While this type of clocking has generated considerable interest in recent years [6, 23, 24], the *design* of such clocking electrodes has, to date, been a highly under-addressed issue in QCA. All work in this area so far has focused on the ability to use electrodes for clocking QCA circuits but has failed to discuss in any detail the sizing, spacing, phase, and applied potential of such electrodes. Moreover, the power consumption of submerged electrodes is assumed to be comparable to that of the QCA devices themselves, which may not necessarily be the case.

1.2 Thesis Overview

The rest of this thesis is organized as follows:

Chapter 2 is broken down into four sections. Section 2.1 provides a general overview of the 3-state QCA technology that will provide the necessary groundwork for the remaining chapters of this thesis. Section 2.2 describes the intra- and inter-cellular energies of the cells in each of the three under-

lying basis configurations. Section 2.3 shows the modelling of the electrodes and their placement with respect to the QCA cell. Section 2.4 describes the electrostatic energy of the cell configuration due to the clocking electrodes.

Chapters 3, 4, and 5 are extracted from a manuscript that has been submitted to "IEEE Transactions on Nanotechnology" [25]. This manuscript investigates the design of clocking infrastructure required for molecular QCA implementations. In Chapter 3, analytical expressions are provided that will help develop limits on the clocking potential and maximum phase difference of adjacent electrodes to ensure the correct functionality of fundamental building blocks in QCA.

Chapter 4 provides simulation results of fundamental building blocks in QCA and shows the dependency of these building blocks on various cell parameters.

In Chapter 5 of this thesis, the temperature dependency of these building blocks is investigated as well as the root-mean-square (RMS) voltages required for correct functionality...

Chapter 6 investigates the effect of random phase shifts on the underlying clock signals in a QCA circuit.

Chapter 2

Theory

2.1 3-State QCA

The fundamental unit in QCA is the QCA cell, created with either 4 or 6 quantum dots and 2 mobile electrons. QCA devices and circuits have been constructed from metallic islands [9, 10, 26–29] and from nano magnets [11–14, 30, 31], but can potentially be made from a single chemical molecule [4, 6, 32]. Molecular QCA offers several advantages over its metal and magnetic counterparts. Firstly, if we consider a molecular QCA cell as a single-molecule device, then QCA circuits can achieve device densities on the order of $10^{14}/\text{cm}^2$ (for 1 nm^2 devices). Current-switched devices such as FETs operating at GHz speeds would melt the chip at those densities. Molecular QCA however has been predicted to reduce the power dissipation by many orders of magnitude [33]. Additionally, the smaller the size, the larger the Coulombic energies of the cell. At the molecular scale, these energies are expected to be in the 0.2–0.5 eV range [2, 3, 34] which allow for room temperature operation since these energies are much greater than the thermal ambient energy $k_B T$ ($\sim 25 \text{ meV}$ at room temperature), where k_B is Boltzmann’s constant and T is the temperature in kelvin ($T = 293 \text{ K}$ at room temperature). Lastly, molecular QCA can be clocked at extremely high frequencies (adiabatically at 1 THz) [33] - much faster than reported speeds of the magnetic QCA cell [2].

2.1.1 Model

In a molecular implementation, the role of quantum dots is played by redox centers within the molecule. A redox center can add an electron (*i.e.*, be reduced) or lose an electron (*i.e.*, be oxidized) without breaking chemical bonds [6, 35]. In particular, two types of redox centers have been investigated - those whose non-bonding orbitals are comprised of mainly s and p states and those whose states are principally comprised of d states from transition metals [4, 6, 32]. Si-phthalocyanine is an example of the former [36] while an example of the latter is the Ru-based Creutz-Taube ion [37].

In the context of this thesis, a simplified model of a molecular QCA cell is investigated in order to reduce the model complexity so that a set of analytical expressions to describe the effect of the clocking electrodes on the ground state of the molecular QCA cell can be developed. A full quantum mechanical model would solve the Schrödinger equation to find the spatial distribution of charge in the molecular orbitals, including spin.

In this thesis, we use a 3-dimensional QCA cell geometry which includes a mechanism for clocking molecular QCA cells proposed in [6, 23, 24], and has been shown to act as a QCA device, switching from a chemical representation of a binary 0 to a binary 1. In this work, the dynamics of these cells are not considered. Instead, only the ground state energies of different cell configurations are determined. In their simplified form, the 3-state QCA cells are composed of "V"-shaped molecules, each with three sites, grouped in pairs. Each pair of molecules represents an individual QCA cell as shown in Figure 2.1. Here, the three basis states of a QCA cell are shown. The sites represent locations in the molecule where the mobile charges can exist and take the role of the quantum dots. Spin and other internal degrees of freedom such as mechanical vibration due to Coulombic forces are not considered in this work.

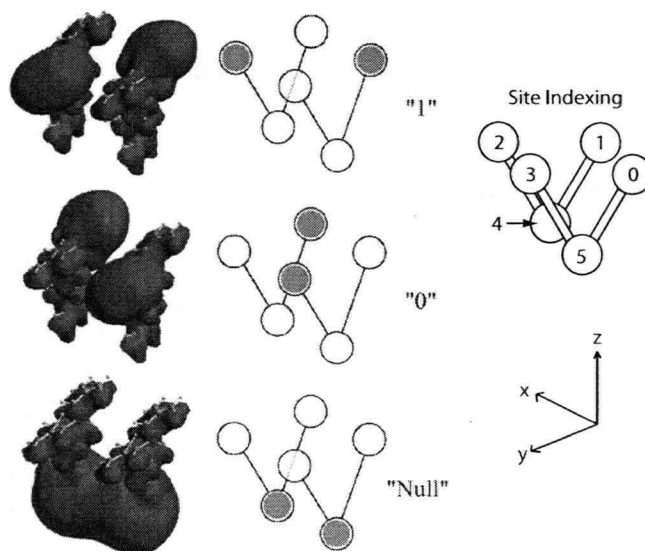


Figure 2.1: 3-state QCA cells are composed of "V"-shaped molecules grouped in pairs [1]. The site indexing used throughout this thesis is indicated in the right figure.

For the molecular QCA cell, three stable electronic configurations are chosen as a basis. Two electronic configurations, in which the mobile charges are located in the top sites of the cell and along one of the two diagonals, represent the ACTIVE states of the cell. In these ACTIVE configurations, the cell is said to have a polarization, $P = \pm 1$. When $P = 1$, the cell is said to represent a binary value of 1, and when $P = -1$, the cell is said to represent a binary value of 0 as shown in Figure 2.1. A circuit-level diagram of a QCA cell is shown in Figure 2.2 depicting the different polarizations of the QCA cell. For simplicity, the bottom two sites are not included. Here, the bounding box around the cell is used only to distinguish one cell from another and has no physical analogue.

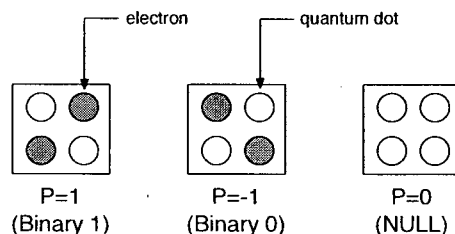


Figure 2.2: Three QCA cells with different polarizations are shown. Each cell carries two extra electrons which tend to occupy the diagonals of the cell when in one of the two ACTIVE states.

When a cell is in one of the two ACTIVE states, its electrostatic interaction with neighbouring cells introduces a perturbation that breaks the energy degeneracy of the active states of the neighbouring cells and in the ground state, adjacent cells tend to relax to the same ACTIVE state as shown in Figure 2.3. In the NULL state, where the cell has a polarization, $P = 0$, the mobile charges are located in the bottom sites of the cell. In this configuration, the cell does not break the energy degeneracy of ACTIVE states in neighbouring cells. Therefore, cells relax to a polarization that is determined only by the interaction with neighbouring cells for which $P \neq 0$.

As a result of the interaction between cells, neighbouring cells will synchronize their polarization. Therefore, an array of QCA cells acts as a wire and is able to transmit information from one end to another; *i.e.*, all the cells in the wire will switch their polarizations to follow that of the input or driver cell as shown in Figure 2.4.

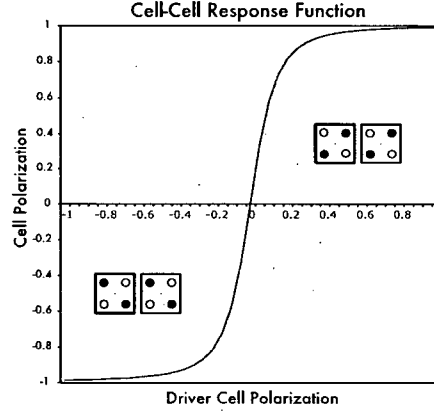


Figure 2.3: Illustration of the non-linear cell-to-cell response function [2]. The non-linear response provides noise margin and signal restoration.

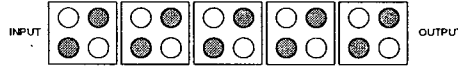


Figure 2.4: A QCA wire is created with a linear array of QCA cells. The cells in the wire will synchronize their polarization to follow the input or driver cell. In this way, information arriving at the input appears at the output after some short propagation delay.

2.1.2 Kink Energy

The Coulombic interactions between two cells can be described by the kink energy, E_k , which describes the energy difference between two cells having different polarizations [38]. The electrostatic interaction between two 6-dot cells m and n can be calculated using,

$$E^{m,n} = \frac{1}{4\pi\epsilon_0\epsilon_r} \sum_{i=0}^5 \sum_{j=0}^5 \frac{Q_i^m Q_j^n}{|r_i^m - r_j^n|}, \quad (2.1)$$

where Q_i^m is the charge at dot i of cell m , r_i^m is the position of dot i in cell m and ϵ_r is the relative permittivity. The kink energy is then determined by calculating the difference in energy between two neighbouring cells having opposite polarization such that,

$$E_k = E_{\text{opposite polarization}}^{m,n} - E_{\text{same polarization}}^{m,n} \quad (2.2)$$

From Equation (2.2), a positive E_k implies that it is energetically favourable for two neighbouring cells to have the same polarization, while a negative E_k suggests that the neighbouring cell will tend to the opposite polarity. The latter result is used to create inversion in QCA circuits.

2.1.3 Computing with QCA

In order to perform general logic computation, a universally complete computing logic set is required. More specifically, we require a set of Boolean logic gates that can perform the AND, OR, and NOT operations. The fundamental logic primitive that can be realized in QCA is the Majority Gate as shown in Figure 2.5. The truth table for the majority gate is shown in Table 2.1.

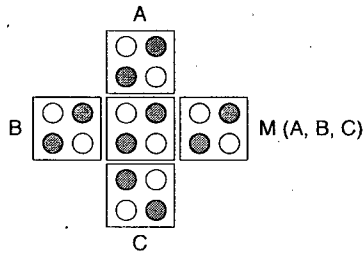


Figure 2.5: QCA majority gate. The output of the majority gate reflects the majority of the inputs.

A	B	C	M(A, B, C)
0	0	0	0
0	0	1	0
0	1	0	0
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1

Table 2.1: Truth Table for Majority Gate.

The output cell of the majority gate assumes the value of the majority of the input cells. In QCA, a 2-input AND or OR gate can easily be created by simply fixing the polarization of one of the three inputs to a logic “0” or a logic “1”, respectively, as shown in Figure 2.6.

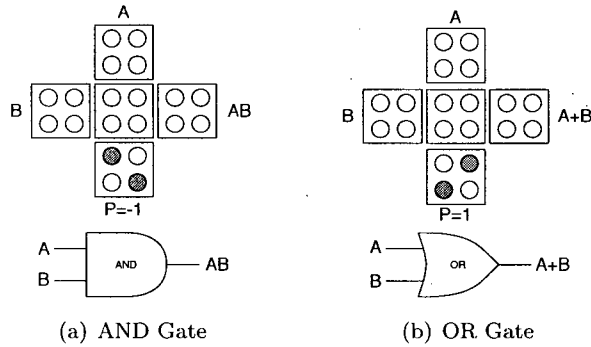


Figure 2.6: Fixing one of the inputs of a majority gate to $P=-1$ creates an AND gate. Similarly, fixing one of the inputs to $P=1$ creates an OR gate.

An inverter can be implemented in QCA by placing cells at 45° angles from one another. At 45° , the kink energy between two cells is negative. As a result, it becomes energetically favourable for two cells in this configuration to take on opposing polarities from one another. Figure 2.7 shows one possible inverter layout and is based on this property.

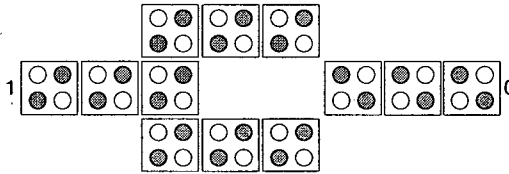


Figure 2.7: QCA inverter. Cells placed at 45° with respect to one another have a negative kink energy between them and hence their polarization is opposite.

Another fundamental circuit is the FANOUT, *i.e.*, one input and two or more outputs (see Figure 2.8). The FANOUT block is also easy to implement, in fact, it is structurally identical to the majority gate.

The only functional difference between the FANOUT and majority gate

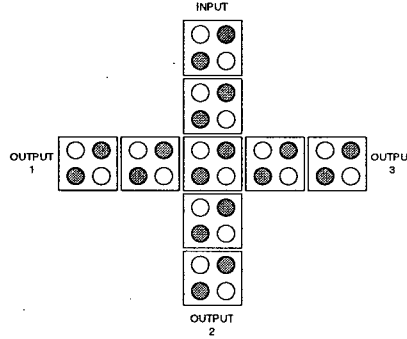


Figure 2.8: An example of QCA fanout. The input appears at each of the three outputs.

building blocks is in the flow of data which is determined by the clock and will be discussed in the next section.

2.1.4 Clocking

Clocking is not only required for the synchronization of information flow in a QCA circuit, but it is also relied upon to deliver power to run the circuit [33]. QCA cells are not powered from any other external source other than the clock, hence the clocking infrastructure is a critical part of the QCA paradigm. Clocking can be implemented with a set of submerged electrodes which generate an electric field at the level of the QCA molecules [22]. The application of phase shifted sinusoids to each of the electrodes creates a travelling wave and induces an electric potential at each of the different sites of the cell. As a result of the electric fields, cells are forced to switch states at the wavefront of this forward moving wave as illustrated in Figure 2.9. Here, the signal applied to each of the four electrodes shown in Figure 2.9 is shifted by ϕ_i as indicated on the electrodes, such that $\phi_1 < \phi_2 < \phi_3 < \phi_4$. A top-view of the time evolution of the QCA cells shown in Figure 2.9 is shown in Figure 2.10.

In other words, when the applied electric field on the cell in the $\hat{y}$ direction, $\vec{E}_y$, is sufficiently large, it will draw the mobile electrons towards the bottom two sites of the cell forcing the cell into the NULL state. Conversely, if the electric field on the electrodes becomes strongly negative, it will drive the electrons to the upper sites of the cell and force it into one of the ACTIVE states. If the field is only somewhat positive or negative, the cell will

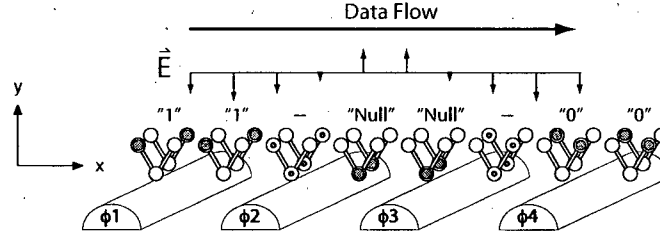


Figure 2.9: Submerged electrodes can be used to clock QCA cells by generating a forward moving electric field at the level of the cells. A ground plane located above the cells is not shown in the figure.

be in a switching state, occupying the upper sites of the cell but still allowed to tunnel through the lower sites and switch its configuration. Which of the cell's upper sites is occupied is not determined by the electric field in the $\hat{y}$ direction, but instead by the quadrupole-quadrupole interactions between neighbouring cells which determine whether a logic "1" or a logic "0" will be represented in the cell.

Note, it is important to recognize that the choice to apply a phase-shifted sinusoidal wave to the electrodes as opposed to a typical square wave is done to ensure that the clock is switched much slower than the tunnelling time between dots, where "tunnelling" is defined as the transitioning through classically-forbidden states. If the cell is switched sufficiently slow, the cell will remain at or close to the ground state at all times, dissipating less energy [22].

2.1.5 Charges

Two fixed positive charges are distributed throughout a cell to ensure that the system is charge neutral. The fraction of neutralizing positive charge located in the top four sites of a cell is determined by the parameter, χ , whose value lies between 0 and 1, and depends on the details of the molecular implementation. Including both mobile and fixed charges, the total charge at each site of a cell for the three basis states can be expressed in a column vector as

$$Q_+ = \left[\chi \frac{e}{2}, \chi \frac{e}{2} - e, \chi \frac{e}{2}, \chi \frac{e}{2} - e, (1 - \chi)e, (1 - \chi)e \right]^T, \quad (2.3)$$

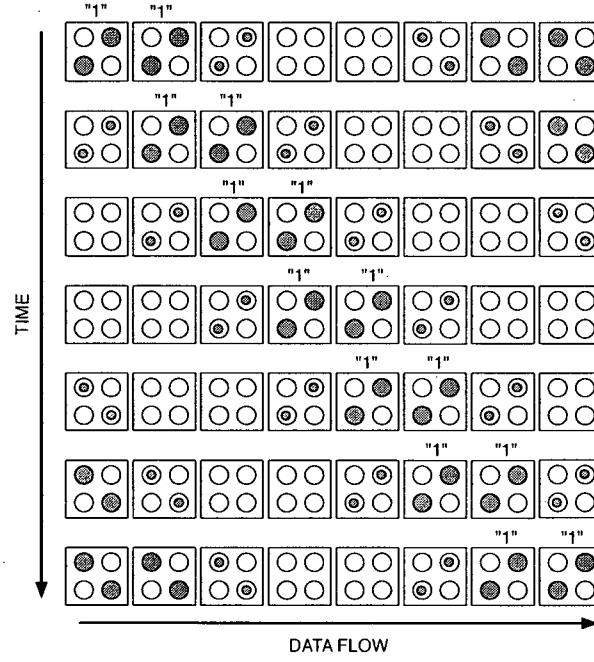


Figure 2.10: A top-view of the time evolution of the QCA cells shown in Figure 2.9. The forward moving wave applied to the electrodes allows for the data to flow in one direction.

$$Q_- = \left[\chi \frac{e}{2} - e, \chi \frac{e}{2}, \chi \frac{e}{2} - e, \chi \frac{e}{2}, (1 - \chi)e, (1 - \chi)e \right]^T, \quad (2.4)$$

and

$$Q_{NULL} = \left[\chi \frac{e}{2}, \chi \frac{e}{2}, \chi \frac{e}{2}, \chi \frac{e}{2}, -e\chi, -e\chi \right]^T, \quad (2.5)$$

where e is the electronic charge of an electron. The elements of these charge vectors are

$$Q = [Q_{\text{site } 0}, Q_{\text{site } 1}, Q_{\text{site } 2}, Q_{\text{site } 3}, Q_{\text{site } 4}, Q_{\text{site } 5}]^T, \quad (2.6)$$

with respect to the indexing shown in Figure 2.1.

2.2 Configuration Energies

Intracellular electrostatic energies are calculated using

$$U_{\kappa}^{intra} = \frac{1}{4\pi\epsilon_0\epsilon_{r1}} \sum_{i=0}^4 \sum_{j=i+1}^5 \frac{Q_{\kappa}(i)Q_{\kappa}(j)}{|r(i) - r(j)|}, \quad (2.7)$$

where $\kappa = \{+, -, NULL\}$ represents one of the three underlying configurations and $|r(i) - r(j)|$ is the distance between sites i and j . The distance between the upper adjacent sites, *i.e.*, sites 0-3, is d , diagonal site separation is therefore $\sqrt{2}d$. The z position of sites 4 and 5 is a distance, α , below the plane of a cell's upper sites. For the purposes of this work, the cell size is defined as the inter-site distance, d . A figure illustrating the QCA cell dimensions is shown in Figure 2.11.

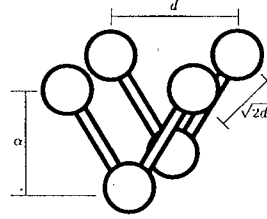


Figure 2.11: QCA cell dimensions.

The electrostatic potential induced by neighbouring cells is computed using

$$V_{\kappa}^m(i) = \frac{1}{4\pi\epsilon_0\epsilon_{r1}} \sum_{j=0}^5 \frac{Q_{\kappa}^m(j)}{|r(i) - r^m(j)|}, \quad (2.8)$$

where $V_{\kappa}^m(i)$ is the potential at the i^{th} site due to neighbouring cell m in basis state, κ , Q_{κ}^m is the charge vector of cell m , and $r^m(j)$ is the position of the j^{th} site of cell m . Using equation (2.8), an expression for the interaction energies between cells n and m can be described by the following [39,40],

$$U_{\kappa_n, \kappa_m}^{inter} = \sum_{m \in \mathbf{N}_c} \sum_{i=0}^5 Q_{\kappa_n}(i) V_{\kappa_m}^m(i), \quad (2.9)$$

where $\mathbf{N}_c$ is the effective neighbourhood of cell n and is defined as all cells existing within a single cell radius of cell n . Here, κ_n and κ_m represent the basis states for cells n and m , respectively.

2.3 Electrodes

As part of this thesis, only two adjacent electrodes are considered and the energetics of a single cell located directly above the mid-point between the electrodes is modelled. This case is considered because the applied potential of the electrodes has the least effect on the middle cell and thus represents the worst-case scenario. As well, the transverse component of the electric field is strongest at the centre of the electrodes and it will be shown in Section 3.2 that this transverse field can lead to unwanted states. The clocking electrodes are modelled as micro-strips whose potential is measured relative to a ground plane located above the layer of cells. The zero potential ground plane is realized in this model using the method of images. Figure 2.12 shows the position of the electrodes and their images, as well as the location of the QCA cell. Here, we do not include a mirror image of the QCA cell as its contribution to the ground plane is negligible and adds unnecessary complexity to the analytical expressions developed later in this thesis.

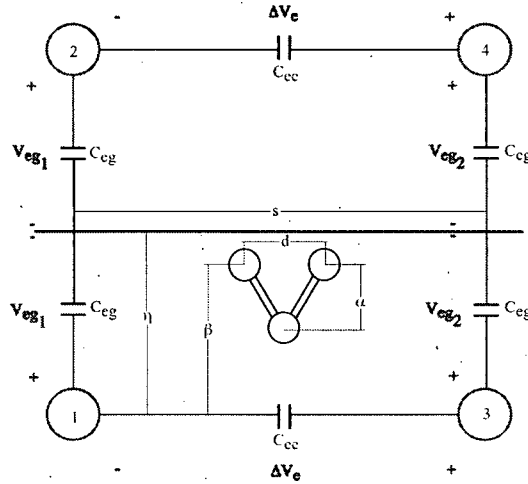


Figure-2.12: Section showing location of the two modelled electrodes (1,3), electrode images (2,4), pseudo-ground plane, and the QCA cell.

Let V_{avg} be the average potential of the electrodes such that $V_{avg} = (V_{eg1} + V_{eg2})/2$, and ΔV_e be the potential difference between adjacent electrodes, then the charge on each of the electrodes can be expressed as a

function of V_{avg} and ΔV_e such that,

$$\begin{aligned} Q_1 &= C_{eg}(V_{avg} - \frac{\Delta V_e}{2}) + C_{ee}(-\Delta V_e), \\ &= -Q_2, \end{aligned} \quad (2.10)$$

$$\begin{aligned} Q_3 &= C_{eg}(V_{avg} + \frac{\Delta V_e}{2}) + C_{ee}(\Delta V_e), \\ &= -Q_4, \end{aligned} \quad (2.11)$$

where C_{eg} is the capacitance between the electrode and the ground plane and is approximated by [41, 42]

$$C_{eg} = l \frac{2.64 \times 10^{-11}(\epsilon_{r2} + 1.41)}{\ln[5.98\eta/(0.8w + t)]}, \quad (2.12)$$

and C_{ee} is the capacitance between neighbouring electrodes and is modelled using the standard result for two parallel cylindrical conductors as

$$C_{ee} = l \frac{\pi \epsilon_0 \epsilon_{r2}}{\cosh^{-1}(\frac{s}{t})}, \quad (2.13)$$

where l , w , and t represent the length, width, and thickness of the electrode, respectively, while s denotes the distance between neighbouring electrodes and η the distance between the ground plane and the electrodes. Here, we also distinguish between the relative permittivity associated with the material between electrodes (ϵ_{r2}) and the one used within the cell (ϵ_{r1}).

2.4 Clocking Energies

For large electrode lengths, *i.e.*, $l \geq 100$ nm, the potential induced at the different sites of a cell can be approximated using the standard result [39, 40]

$$V_{clk}(i) = \sum_{j \in \mathbf{N}_e} \frac{\rho_j}{2\pi \epsilon_0 \epsilon_{r2}} \ln |\vec{r}_i|, \quad (2.14)$$

where $\mathbf{N}_e$ is the neighbourhood of nearest adjacent electrodes, $|\vec{r}_i|$ is the distance from the location of the i^{th} site to the electrode, and ρ_j is the charge density of the electrode, which is determined by dividing the total charge on the electrode by its total length, l . The total electrostatic energy of the cell configuration due to the clocking electrodes is

$$U_{\kappa}^{clk} = \sum_{i=0}^5 V_{clk}(i) Q_{\kappa}(i). \quad (2.15)$$

Chapter 2. Theory

The application of this clocking field does not introduce any perturbation between the two ACTIVE states. However, the clock will introduce an energy difference between the NULL and ACTIVE states, permitting us to use the clock to switch the cell between the ACTIVE and NULL state.

Chapter 3

Functional Analysis of a QCA Cell

In this chapter, the effect of applied potential, potential difference between electrodes, and electrode spacing on the different possible configurations of a cell placed directly above the mid-point between two identical electrodes is investigated to determine a set of operational ranges for these parameters.

3.1 ACTIVE to NULL

Here, the energy of the ACTIVE and NULL states of the cell is analyzed with respect to the different applied clocking potentials in order to determine if such potentials are sufficient to switch the cell between these two states. The total electrostatic energy for the ACTIVE and NULL states is given by,

$$\begin{aligned} U_{ACTIVE} &= U_{ACTIVE}^{intra} + U_{ACTIVE}^{clk} + U_{ACTIVE, \kappa_m}^{inter}, \\ U_{NULL} &= U_{NULL}^{intra} + U_{NULL}^{clk} + U_{NULL, \kappa_m}^{inter}. \end{aligned} \quad (3.1)$$

We are interested in the difference between these two energies; *i.e.*,

$$\begin{aligned} \Delta U_{NA} &= U_{NULL} - U_{ACTIVE} \\ &= \Delta U_{NA}^{intra} + \Delta U_{NA}^{clk} + \Delta U_{NA}^{inter}. \end{aligned} \quad (3.2)$$

From the above, it follows that while ΔU_{NA} is positive, the cell will tend to the ACTIVE state since it represents the lower energy state, and when negative, tend to the NULL state. Using equations (2.7) and (2.15), ΔU_{NA}^{intra} and ΔU_{NA}^{clk} can be reduced to

$$\begin{aligned} \Delta U_{NA}^{intra} &= \frac{d(-2 + \sqrt{2}(-1 + \chi) + 8\chi)}{8d^2\pi\epsilon_0\epsilon_{r1}} \\ &\quad - e^2 \frac{(8d^2\sqrt{4\alpha^2 + d^2} + \sqrt{4\alpha^2 + 5d^2})(-1 + 2\chi)}{8d^2\pi\epsilon_0\epsilon_{r1}\sqrt{4\alpha^2 + d^2}\sqrt{4\alpha^2 + 5d^2}}, \end{aligned} \quad (3.3)$$

$$\Delta U_{NA}^{clk} = -eV_{avg} \frac{C_{eg}(\gamma_1 + \gamma_2 - \gamma_3 - \gamma_4 - 2(\gamma_5 - \gamma_6))}{4l\pi\epsilon_0\epsilon_{r2}}, \quad (3.4)$$

where each of the γ_i terms can be constructed using

$$\begin{aligned} \gamma_1 &= \ln[\beta^2 + \frac{1}{4}(d-s)^2] \\ \gamma_2 &= \ln[\beta^2 + \frac{1}{4}(d+s)^2] \\ \gamma_3 &= \ln[(\beta - 2\eta)^2 + \frac{1}{4}(d-s)^2] \\ \gamma_4 &= \ln[(\beta - 2\eta)^2 + \frac{1}{4}(d+s)^2] \\ \gamma_5 &= \ln[(\beta - \alpha)^2 + \frac{s^2}{4}] \\ \gamma_6 &= \ln[(-\beta + \alpha + 2\eta)^2 + \frac{s^2}{4}], \end{aligned}$$

where α is the cell height, β is the distance between the cell and the plane of the electrodes, and η is the distance between the electrode and ground plane.

The ΔU_{NA}^{inter} term will be expanded in the later sections of this work.

3.2 ACTIVE to X

The assumption that the cell can only exist in one of three underlying basis states requires that $\vec{E}_x$, *i.e.*, the field across the cell, be sufficiently low that the two mobile charges not both accumulate at one side of the cell. These higher energy states, sometimes called “X” states, are shown in Figure 3.1. If cells are permitted to go into such states, data will be lost and the circuit will fail to operate properly. The following analysis is performed in order to define a maximum potential difference between adjacent electrodes to ensure that cells not reach these unwanted states.

The charge vectors associated with the two unwanted X states are as follows

$$Q_{X1} = \left[x\frac{e}{2} - e, x\frac{e}{2} - e, x\frac{e}{2}, x\frac{e}{2}, (1-x)e, (1-x)e \right]^T, \quad (3.5)$$

$$Q_{X2} = \left[x\frac{e}{2}, x\frac{e}{2}, x\frac{e}{2} - e, x\frac{e}{2} - e, (1-x)e, (1-x)e \right]^T. \quad (3.6)$$

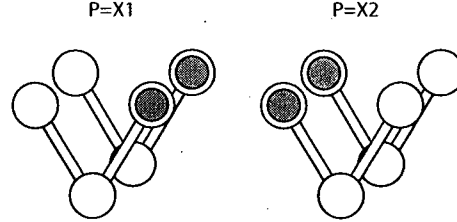


Figure 3.1: When the mobile charges are both located on the same side of the cell, the cell is said to be in one of the unwanted X states.

Whether or not the cell tends to one of these two states can be determined by first evaluating the difference in clocking energies for both the ACTIVE and X state, then adding this to the difference in their intracellular energies. The lowest energy difference, and hence the highest probability of accessing one of these X states, can be approximated with a single cell while neglecting the effect of neighbouring cells. To justify the latter claim, consider the 3-cell wire shown in Figures 3.2(a) and 3.2(b). Figure 3.2(a) shows a strong electric field, E_f , acting on the three cells as indicated by the arrows. For the cells 2 and 3 to revert to an X state, both would need to overcome the Coulombic repulsion due to the electrons in their own cells as well as from the neighbouring cell to their left. The lower-left electron in cell 1, however, would need only enough energy to overcome the Coulombic repulsion due to the electron in its own cell, *i.e.*, the effect of electrons in the neighbouring cell can be neglected. Thus, cell 1 in the 3-cell wire would be the first to revert to an X state as shown in Figure 3.2(b).

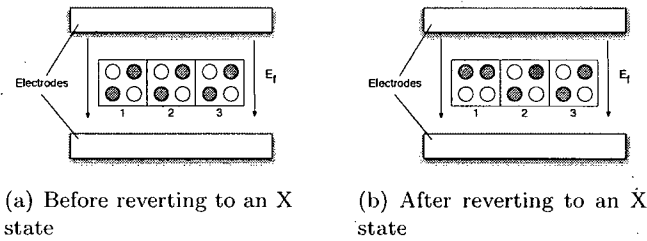


Figure 3.2: The switching of a cell from an ACTIVE to X state for a 3-cell wire.

Given a single cell, the energy difference between X and ACTIVE states

is

$$\Delta U_{XA}^{intra} = -e^2 \frac{(-2 + \sqrt{2})(-2 + \chi)^2}{32d\pi\epsilon_0\epsilon_{r_1}} \quad (3.7)$$

$$\Delta U_{XA}^{clk} = \pm e\Delta V_e \frac{(C_{eg} + 2C_{ee})(\gamma_1 - \gamma_2 - \gamma_3 + \gamma_4)}{4l\pi\epsilon_0\epsilon_{r_2}} \quad (3.8)$$

where the “ $\pm$ ” represents the equal and opposite nature of the ΔU_{XA}^{clk} terms with respect to the two X states.

3.3 Maximum Phase Difference

For a given configuration of clocking electrodes and cell geometry, the above analysis can be used to determine maximum and minimum values for ΔV_e . This information can further be used to determine the maximum phase difference between neighbouring electrodes which ensures that the transverse electric field intensity does not cause the cell to relax into one of these unwanted states as

$$\phi_{max} = \pm 2 \sin^{-1} \left(\frac{\Delta V_{e_{max}}}{2V_0} \right) \text{ radians}, \quad (3.9)$$

where V_0 is the peak potential of the phase shifted sinusoid applied to the electrodes.

It is desirable to achieve large values for ϕ_{max} so that the total number of clocking phases required for correct operation of a QCA circuit can be kept as low as possible. Previous work has used 4 phases to clock QCA circuits.

Chapter 4

Simulations (including results)

In this section, three potential scenarios are considered for simulation to estimate operational ranges for the placement, applied potential, and relative phase between adjacent electrodes:

1. A single QCA cell placed directly at the mid-point between two identical electrodes (see Figure 4.1(a));
2. A 3-cell wire with the middle cell placed at the mid-point between two identical electrodes (see Figure 4.1(b));
3. A 3-input majority gate with the middle cell placed at the mid-point between two identical electrodes (see Figure 4.1(c)).

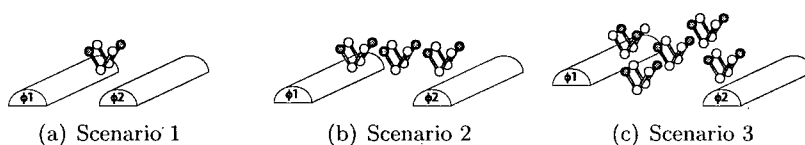


Figure 4.1: 3 simulated scenarios.

For each simulation, $\chi = 0.5$ unless otherwise specified, and the relative permittivities inside and between cells (ϵ_{r1}) and in between the electrodes and molecules (ϵ_{r2}) are chosen to be 1 and 12.9, respectively. The choice for ϵ_{r2} is based on the assumption that the electrodes will be placed under a semiconductive material. Given that the substrate material is not yet known, this value serves only as an approximation and does not necessarily represent the properties of future QCA implementations.

Both the ΔU_{NA}^{intra} and ΔU_{NA}^{clk} terms remain unchanged for all three scenarios since we are only considering the different possible configurations on the middle cell, which remains in the same location relative to the electrodes.

4.1 Single Cell

4.1.1 ACTIVE to NULL

In a first set of simulations, a single cell with size $d = 1$ nm and a cell height of $\alpha = 1.2$ nm is considered. The electrodes are placed at a distance $\eta = 10$ nm below the ground plane and the cells placed $\beta = 2.8$ nm above the electrodes. An electrode length, $l = 100$ nm, width, $w = 1$ nm, and thickness, $t = 1$ nm, were chosen. Here, the potential on the electrodes is kept equal, *i.e.*, $\Delta V_e = 0$. Figure 4.2 plots equation (3.2) and shows the minimum electrode potential required to switch the cell from an ACTIVE to a NULL state for three values of χ as a function of the electrode spacing, s . From Figure 4.2, to switch a 1 nm cell with a χ value of 0.5 placed between two electrodes spaced 10 nm apart, an average electrode potential of at least 10 V is required.

The cell sizing can significantly impact the switching potential of the clocking electrodes. Figure 4.3 shows the change in V_{avg} as the distance between adjacent electrodes is increased for three different cell sizes. From the figure, the switching potential increases as the cell sizes decrease. This is expected since the clock needs to overcome the increased contribution from intra- and inter-cellular energies due to the increased proximity of the mobile electrons in the cell.

4.1.2 ACTIVE to X

For a second set of simulations, the values of d , α , β and η as well as the electrode dimensions were kept the same as they were for the first simulation. The potential difference between the electrodes, ΔV_e , was plotted while maintaining V_{avg} constant. Figure 4.4 shows ΔV_e as a function of the electrode spacing for three different values of χ . The two diverging curves for each value of χ represent the maximum voltage differences between the electrodes before the X states become energetically favourable. The value of ΔV_e is important because it provides insight on the maximum allowable phase difference between sinusoids applied between two neighbouring electrodes. Figure 4.5 shows the change in the maximum value of ΔV_e as a

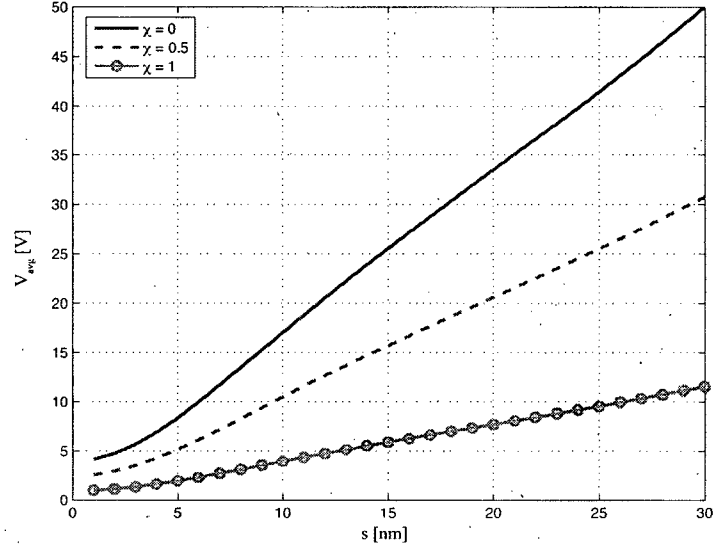


Figure 4.2: Switching potential vs electrode spacing of a 1 nm cell for 3 different values of χ .

function of the electrode spacing for various cell sizes. The plot shows that the minimum potential difference needed to force a cell into one of the X states increases as the cell size is decreased. This is due to the increased intra-cellular energies of the cell.

4.2 3-Cell Wire

Two different wire configurations were set up as shown in Figures 4.6(a) and 4.6(b). Figure 4.6(a) represents the worst-case scenario for turning the middle cell “on” while Figure 4.6(b) represents the worst-case scenario for switching the middle cell “off”. Intuitively, one might expect that the worst-case scenario to switch a cell “on” would feature two cells of opposite polarity along the same wire. However, realistically, two opposite cells would never appear in a wire unless the wire was part of a majority gate which is considered in Section 4.3. For such wire, the potential for the centre cell to go into one of the X states is not considered here again since the worst case scenario for this has already been addressed.

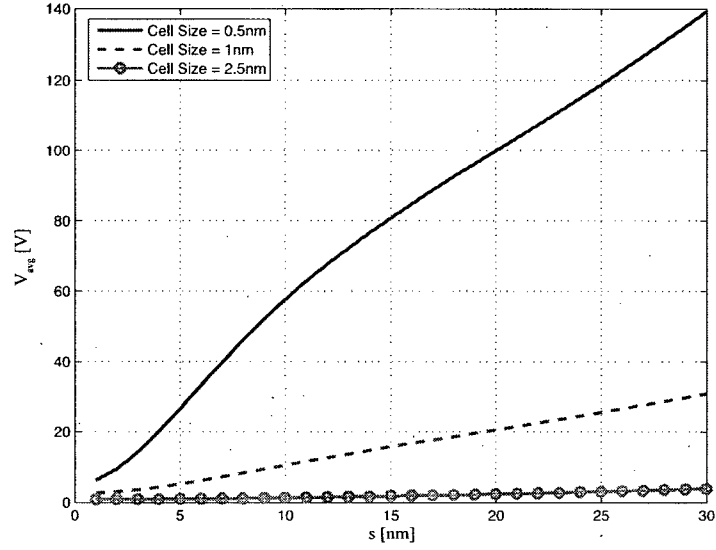


Figure 4.3: Switching potential vs the electrode spacing for 0.5 nm, 1 nm, and 2.5 nm cells.

Figure 4.6(a) shows a cell in between two active cells, while Figure 4.6(b) shows the same cell in between two cells in the NULL state. For Figure 4.6(a), the interaction energy can be expressed as,

$$\begin{aligned}
 U_{NULL, \kappa_m}^{inter_{w1}} &= \sum_{i=0}^5 Q_{NULL}^n(i) V_{\kappa_{n+1}}^{n+1}(i) \\
 &\quad + \sum_{i=0}^5 Q_{NULL}^n(i) V_{\kappa_{n-1}}^{n-1}(i) \\
 &= \sum_{i=0}^5 Q_{NULL}^n(i) V_{ACTIVE}^{n+1}(i) \\
 &\quad + \sum_{i=0}^5 Q_{NULL}^n(i) V_{ACTIVE}^{n-1}(i)
 \end{aligned} \tag{4.1}$$

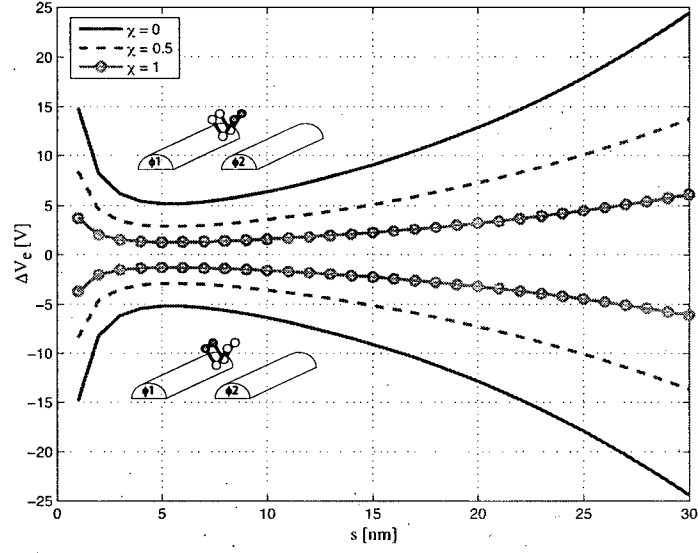


Figure 4.4: Maximum allowable ΔV_e before reverting to an X state for a 1 nm cell for 3 different values of χ .

$$\begin{aligned}
 U_{ACTIVE, \kappa_m}^{inter_{w1}} &= \sum_{i=0}^5 Q_{ACTIVE}^n(i) V_{\kappa_{n+1}}^{n+1}(i) \\
 &\quad + \sum_{i=0}^5 Q_{ACTIVE}^n(i) V_{\kappa_{n-1}}^{n-1}(i) \\
 &= \sum_{i=0}^5 Q_{ACTIVE}^n(i) V_{ACTIVE}^{n+1}(i) \\
 &\quad + \sum_{i=0}^5 Q_{ACTIVE}^n(i) V_{ACTIVE}^{n-1}(i). \tag{4.2}
 \end{aligned}$$

However, due to symmetry, equations (4.1) and (4.2) reduce to

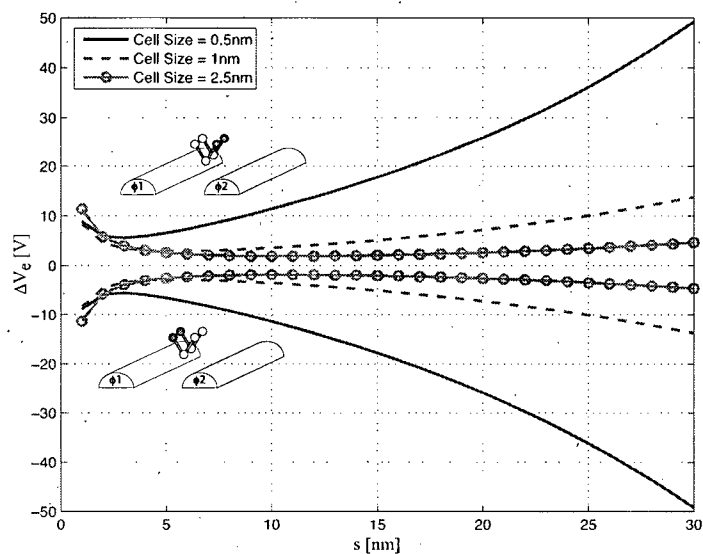


Figure 4.5: Maximum potential difference allowable before reverting to an X state for 0.5 nm, 1 nm, and 2.5 nm cells vs. the distance between adjacent clocking electrodes.

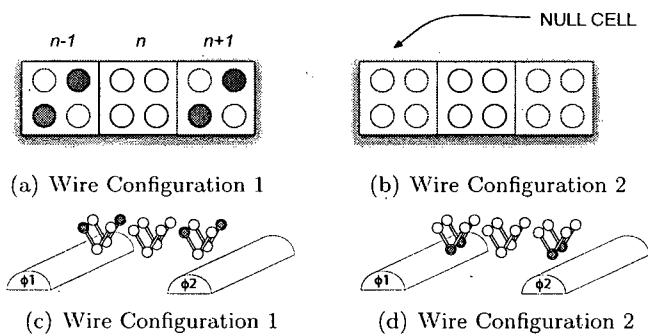


Figure 4.6: Wires representing the maximum and minimum potentials for switching the middle cell. Molecular representations are shown in (c) and (d). Cell indexing is shown in (a).

$$U_{NULL,\kappa_m}^{inter_{w1}} = 2 \sum_{i=0}^5 Q_{NULL}^n(i) V_{ACTIVE}^{n+1}(i), \quad (4.3)$$

$$U_{ACTIVE,\kappa_m}^{inter_{w1}} = 2 \sum_{i=0}^5 Q_{ACTIVE}^n(i) V_{ACTIVE}^{n+1}(i). \quad (4.4)$$

The difference in state energies becomes

$$\Delta U_{NA}^{inter_{w1}} = U_{NULL,\kappa_m}^{inter_{w1}} - U_{ACTIVE,\kappa_m}^{inter_{w1}}. \quad (4.5)$$

Similarly, the interaction energies for Wire configuration 2 can be defined as,

$$U_{NULL,\kappa_m}^{inter_{w2}} = 2 \sum_{i=0}^5 Q_{NULL}^n(i) V_{NULL}^{n+1}(i), \quad (4.6)$$

$$U_{ACTIVE,\kappa_m}^{inter_{w2}} = 2 \sum_{i=0}^5 Q_{ACTIVE}^n(i) V_{NULL}^{n+1}(i), \quad (4.7)$$

for which the energy difference becomes

$$\Delta U_{NA}^{inter_{w2}} = U_{NULL,\kappa_m}^{inter_{w2}} - U_{ACTIVE,\kappa_m}^{inter_{w2}}. \quad (4.8)$$

Figure 4.7 plots equation (3.2) for both wire configurations, as a function of the average potential, V_{avg} , for cell sizes of 1 nm. All cell parameters are the same as for the single-cell simulations. From the plot, a V_{avg} of at least 21V is required to ensure that the cell can be forced into the NULL state. Conversely, to guarantee that a cell be turned on, the average electrode potential needs to be brought down below 3V. This represents the minimum range of potential that must be applied to ensure the correct operation of the wire.

4.3 Majority Gate

Similar to the analysis of the wire, two different majority gate (MG) configurations in Figures 4.8(a) and 4.8(b) have been set up to evaluate the maximum and minimum potential applied to the electrodes to ensure that the middle cell (cell 1) can be switched between the ACTIVE and NULL states.

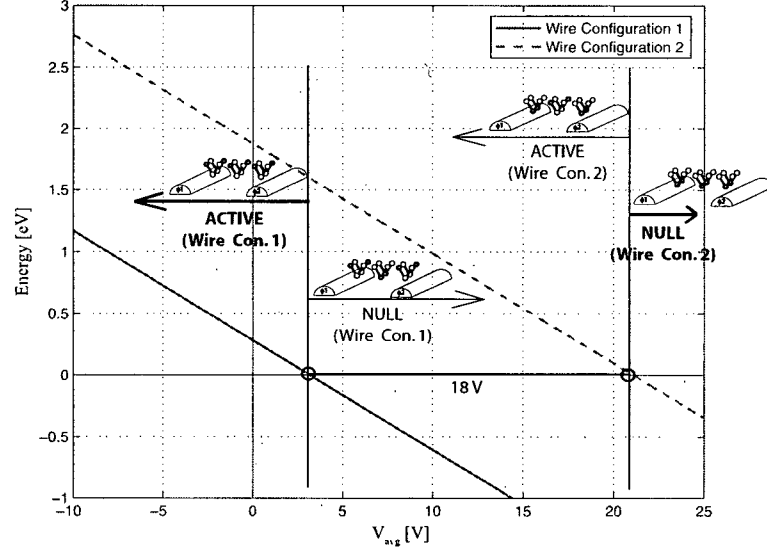


Figure 4.7: ΔU_{NA} vs V_{avg} for two wire configurations using 1 nm cells, which shows that the applied potential range of the electrodes must be at least 18V for correct operation.

MG configuration 1 shows a majority gate with two of its inputs in the $P = +1$ state and the third in the $P = -1$ state, while MG configuration 2 shows all three inputs in the NULL state. For configuration 1, the order of the inputs does not matter, nor does the state of the opposing cell (*i.e.*, a majority gate with two of its inputs in the $P = -1$ state and the third in the $P = +1$ state would yield the same results by symmetry). The output remains in the NULL state for both configurations since it is assumed the clocking wave has not yet reached cell 5. For MG configuration 1, the interaction energies can be expressed as

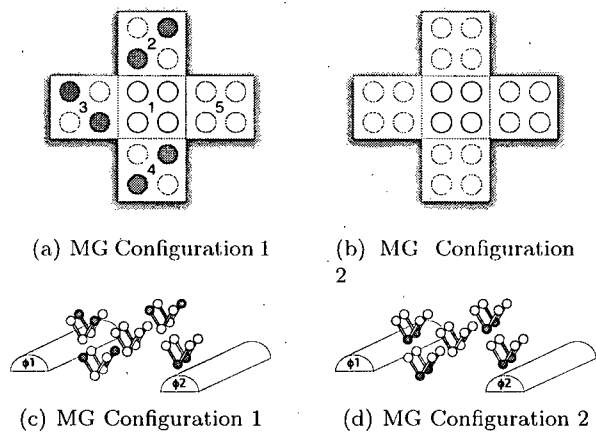


Figure 4.8: Majority Gates representing the worst-case scenarios for switching the middle cell. Molecular representations are shown in (c) and (d). Cell indexing is shown in (a).

$$\begin{aligned}
 U_{NULL, \kappa_m}^{inter_{mg1}} &= \sum_{i=0}^5 Q_{NULL}^1(i) V_+^2(i) \\
 &\quad + \sum_{i=0}^5 Q_{NULL}^1(i) V_-^3(i) \\
 &\quad + \sum_{i=0}^5 Q_{NULL}^1(i) V_+^4(i) \\
 &\quad + \sum_{i=0}^5 Q_{NULL}^1(i) V_{NULL}^5(i), \tag{4.9}
 \end{aligned}$$

$$\begin{aligned}
 U_{ACTIVE, \kappa_m}^{inter_{mg1}} &= \sum_{i=0}^5 Q_+^1(i) V_+^2(i) + \sum_{i=0}^5 Q_+^1(i) V_-^3(i) \\
 &\quad + \sum_{i=0}^5 Q_+^1(i) V_+^4(i) + \sum_{i=0}^5 Q_+^1(i) V_{NULL}^5(i). \tag{4.10}
 \end{aligned}$$

However, due to the symmetry of the majority gate, equations (4.9) and (4.10) can be simplified such that

$$\begin{aligned}
 U_{NULL,\kappa_m}^{inter_{mg1}} &= 2 \sum_{i=0}^5 Q_{NULL}^1(i) V_+^2(i) \\
 &\quad + \sum_{i=0}^5 Q_{NULL}^1(i) V_-^3(i) \\
 &\quad + \sum_{i=0}^5 Q_{NULL}^1(i) V_{NULL}^5(i), \tag{4.11}
 \end{aligned}$$

$$\begin{aligned}
 U_{ACTIVE,\kappa_m}^{inter_{mg1}} &= 2 \sum_{i=0}^5 Q_+^1(i) V_+^2(i) + \sum_{i=0}^5 Q_+^1(i) V_-^3(i) \\
 &\quad + \sum_{i=0}^5 Q_+^1(i) V_{NULL}^5(i). \tag{4.12}
 \end{aligned}$$

The difference in state energies becomes

$$\Delta U_{NA}^{inter_{mg1}} = U_{NULL,\kappa_m}^{inter_{mg1}} - U_{ACTIVE,\kappa_m}^{inter_{mg1}}. \tag{4.13}$$

By making use of the symmetry of the majority gate, the interaction energies for MG configuration 2 can be written as,

$$U_{NULL,\kappa_m}^{inter_{mg2}} = 4 \sum_{i=0}^5 Q_{NULL}^1(i) V_{NULL}^2(i), \tag{4.14}$$

$$U_{ACTIVE,\kappa_m}^{inter_{mg2}} = 4 \sum_{i=0}^5 Q_{ACTIVE}^1(i) V_{NULL}^2(i), \tag{4.15}$$

such that their difference in energy becomes

$$\Delta U_{NA}^{inter_{mg2}} = U_{NULL,\kappa_m}^{inter_{mg2}} - U_{ACTIVE,\kappa_m}^{inter_{mg2}}. \tag{4.16}$$

Figure 4.9 plots equation (3.2) for both majority gate configurations, as a function of the average potential, V_{avg} , for cell sizes of 1 nm. Again, the cell parameters are kept the same as in previous simulations.

In Figure 4.9, it can be seen that the difference between the minimum and maximum electrode potentials is larger for the majority gate than the wire. For the same 1 nm cells, the minimum average potential required to force the cell into the NULL state jumps from 21V in the case of the wire to about 32V for the majority gate, and the maximum allowed average potential to keep a cell in the ACTIVE state lowers to -3V - down 6V from the wire. Thus, the minimum range of electrode potentials is determined by considering the majority gate and not the wire. For design purposes, it is important to be able to determine *a priori* the minimum required potential difference between the electrodes. Let ΔU_{NA} for majority gate configurations 1 and 2 be denoted by $\Delta U_{NA_{mg1}}$ and $\Delta U_{NA_{mg2}}$, respectively. To determine the minimum required potential difference between electrodes, we can set both $\Delta U_{NA_{mg1}}$ and $\Delta U_{NA_{mg2}}$ to zero, solve for V_{avg} for both cases, and then subtract the two potentials. Analytically, this can be accomplished if the $\Delta U_{NA_{mg1}}$ and $\Delta U_{NA_{mg2}}$ terms are expressed as

$$\Delta U_{NA_{mg1}} = \Delta U_{NA_{mg1}}^{intra} + \Delta U_{NA_{mg1}}^{inter} + \Delta U_{NA_{mg1}}^{clk}, \quad (4.17)$$

$$= A + \zeta V_{avg1}, \quad (4.18)$$

$$\Delta U_{NA_{mg2}} = \Delta U_{NA_{mg2}}^{intra} + \Delta U_{NA_{mg2}}^{inter} + \Delta U_{NA_{mg2}}^{clk}, \quad (4.19)$$

$$= B + \zeta V_{avg2}, \quad (4.20)$$

where A and B are equal to the sum of the ΔU_{NA}^{intra} (eqn. (3.3)) and ΔU_{NA}^{inter} (eqns. (4.13), (4.16)) terms for configurations 1 and 2, respectively. The clocking energy terms (eqn. (3.4)) for both configurations grow linearly with respect to V_{avg} , and hence can be expressed as ζV_{avg} . Setting both (4.18) and (4.20) to zero, isolating V_{avg1} and V_{avg2} , and subtracting them from one another yields

$$V_{avg2} - V_{avg1} = \frac{A - B}{\zeta} \quad (4.21)$$

$$= \Delta V_{avg}. \quad (4.22)$$

Using equations (4.18), (4.20) and (4.21), ΔV_{avg} can be plotted as a function of the electrode spacing for three different values of χ as shown in Figure 4.10. From Figure 4.10, for a 1 nm cell, as the distance in between neighbouring electrodes is increased, the minimum range for the average electrode potential increases significantly.

The above analysis can also be used to determine what the minimum cell size has to be to in order to satisfy certain layout conditions. For

example, if we wanted to use electrodes with peak potentials of $\pm 5V$ spaced 15 nm apart, then equations (4.17) and (4.19) can be used to determine the minimum allowable cell sizes to meet these conditions for different values of χ . E.g., for $\chi = 0$, a minimum cell size of 2 nm is required, for $\chi = 0.5$, a cell size of 2.6 nm, and for $\chi = 1$, the cell can be no smaller than 3.1 nm. Had a cell size of 2 nm been maintained for each value of χ , then an electrode potential of over 9V would have been required to turn off the cell for $\chi = 0.5$ and no less than 13V to turn off the cell with $\chi = 1$ - much larger than the peak potential of 5V applied to the electrodes. This result suggests that as the value of χ is increased, the switching voltage also increases for a given cell size. However, this contradicts an earlier finding in the case of the single cell, where we were able to *decrease* the switching voltage as we increased the value of χ (Figure 4.2). To understand why this occurs, we need to first recognize the dependence of each of the energy terms on χ . First, from equation (3.4) the difference in clocking energies of a given cell, ΔU_{NA}^{clk} , is not a function of χ . Second, while it is not immediately obvious from equation (3.3), the ΔU_{NA}^{intra} term decreases as the value of χ is increased. Hence, for a single cell, the net effect of these two terms is a decrease in energy with respect to an increase in χ , resulting in a smaller switching potential. Conversely, the difference in intercellular energies, ΔU_{NA}^{inter} , increases with χ . In fact, ΔU_{NA}^{inter} increases faster with χ than ΔU_{NA}^{intra} decreases, and hence the net effect, once ΔU_{NA}^{inter} is included, is that the energy increases with increasing χ . Therefore, this increase in energy results in a larger switching potential for the middle cell.

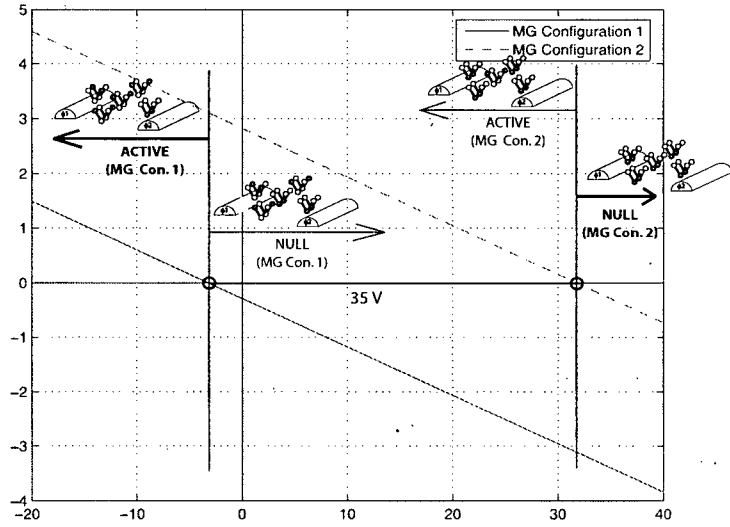


Figure 4.9: ΔU_{NA} vs V_{avg} for two majority gate configurations using 1 nm cells, which shows that the applied potential range of the electrodes must be at least 35V for correct operation.

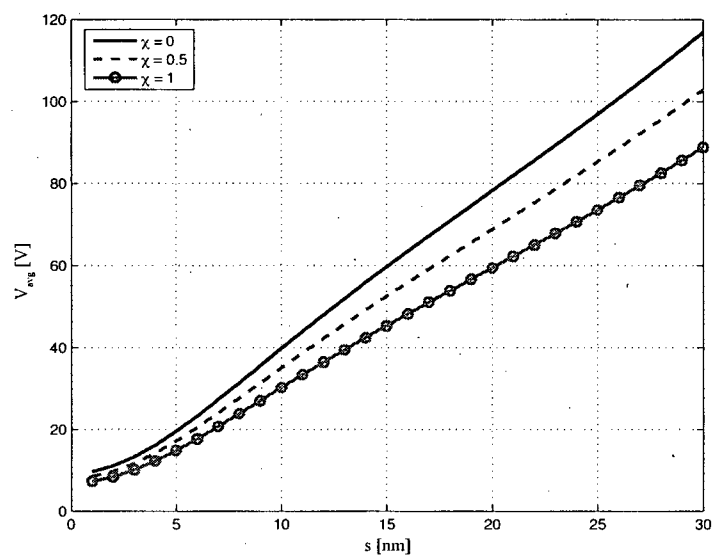


Figure 4.10: Minimum applied potential range of the electrodes for the majority gate vs. the electrode spacing, s , for three different values of χ . Cell sizes of 1 nm were used.

Chapter 5

Temperature Dependency

The preceding simulations assumed a temperature of 0 K. However, if we want to consider the functionality of these building blocks at finite temperatures, then the thermal energy given by $k_B T$ must also be considered, where k_B represents Boltzmann's constant and T is the absolute temperature. To account for this, a statistical thermodynamic model for a QCA cell proposed in [34,43,44] is used. Using this model, the circuit configuration probabilities can be evaluated. Classically, a QCA circuit can be in one of many possible configurations, labelled, j , each with its associated total energy E_j . The expressions required to produce E_j have already been developed in previous chapters. Using the information of the possible states of the system, the canonical partition function in [34]

$$Z = \sum_j \exp\left(\frac{-E_j}{k_B T}\right), \quad (5.1)$$

can be used to compute the state probability for a particular state, i , at a given temperature as

$$P_i = \frac{\exp\left(\frac{-E_i}{k_B T}\right)}{Z}. \quad (5.2)$$

5.1 Majority Gate

In this work, two majority gate configurations have been considered. These represent the worst-case scenarios for switching the middle cell as shown in Figure 4.8. Recall, that it is the majority gate that determines the operational ranges of the clocking electrodes and not the wire. First, consider the configuration presented in Figure 4.8(a). To calculate Z , all the energies associated with each of the possible configurations of the middle cell need to be summed up. Here, the middle cell can be in any of the five ($\kappa = +, -, \text{NULL}, \text{X1}, \text{X2}$) basis states as described in previous chapters. However, for the configurations presented in this thesis, if we choose the “-” state as the ACTIVE state, then the “+” and X states represent energy states that

are much greater than the “-” and NULL states and become negligible in the calculations of the state probabilities. Therefore, Z can be approximated by computing the energies of “-” and NULL states only such that

$$Z_1 \simeq \exp\left(\frac{-E_{ACTIVE_{mg1}}}{k_B T}\right) + \exp\left(\frac{-E_{NULL_{mg1}}}{k_B T}\right), \quad (5.3)$$

where $E_{ACTIVE_{mg1}}$ and $E_{NULL_{mg1}}$ describe the energies of the middle cell in MG configuration 1 being in the ACTIVE and NULL state, respectively. These two energies can be expressed as

$$E_{ACTIVE_{mg1}} = U_{ACTIVE}^{intra} + U_{ACTIVE}^{inter_{mg1}} + U_{ACTIVE}^{clk}, \quad (5.4)$$

$$E_{NULL_{mg1}} = U_{NULL}^{intra} + U_{NULL}^{inter_{mg1}} + U_{NULL}^{clk}, \quad (5.5)$$

where $U_{NULL}^{inter_{mg1}}$ and $U_{ACTIVE}^{inter_{mg1}}$ represent the intercellular energies for MG configuration 1 (equations (4.11) and (4.12), respectively). Here, U_{ACTIVE}^{intra} , U_{NULL}^{intra} , U_{ACTIVE}^{clk} and U_{NULL}^{clk} are identical for both configurations of the majority gate. By substituting equation (5.3) into (5.2), the probability that the middle cell will be in either the ACTIVE or NULL state can be expressed as

$$P_{ACTIVE_1} = \frac{\exp\left(\frac{-E_{ACTIVE_{mg1}}}{k_B T}\right)}{Z_1}, \quad (5.6)$$

$$P_{NULL_1} = \frac{\exp\left(\frac{-E_{NULL_{mg1}}}{k_B T}\right)}{Z_1}. \quad (5.7)$$

Similarly, the state probabilities for the middle cell can be computed for the configuration shown in Figure 4.8(b) by simply modifying equations (5.3), (5.4) and (5.5) such that,

$$Z_2 \simeq \exp\left(\frac{-E_{ACTIVE_{mg2}}}{k_B T}\right) + \exp\left(\frac{-E_{NULL_{mg2}}}{k_B T}\right), \quad (5.8)$$

and

$$E_{ACTIVE_{mg2}} = U_{ACTIVE}^{intra} + U_{ACTIVE}^{inter_{mg2}} + U_{ACTIVE}^{clk}, \quad (5.9)$$

$$E_{NULL_{mg2}} = U_{NULL}^{intra} + U_{NULL}^{inter_{mg2}} + U_{NULL}^{clk}. \quad (5.10)$$

Then, the state probabilities for the middle cell of MG configuration 2 becomes

$$P_{ACTIVE_2} = \frac{\exp(\frac{-E_{ACTIVE_{mg2}}}{k_B T})}{Z_2}, \quad (5.11)$$

$$P_{NULL_2} = \frac{\exp(\frac{-E_{NULL_{mg2}}}{k_B T})}{Z_2}. \quad (5.12)$$

These state probabilities can be used to determine, within a certain likelihood, what RMS voltage is required for correct functionality of a QCA circuit. Let V_1 be the maximum allowable V_{avg} to keep a cell in the ACTIVE state and V_2 be the minimum allowable V_{avg} to force a cell into the NULL state. Then we can define V_{rms} as $\sqrt{(V_1^2 + V_2^2)/2}$. For a given cell size and statistical probability, equations (5.6) and (5.12) can be used to compute the values of V_1 and V_2 , respectively, as well as the maximum operational temperature. Figure 5.1 plots both the minimum V_{rms} required and the maximum operational temperature allowed versus cell size such that the statistical probability of success is 99%. Equation (3.9) was also used to plot the maximum allowable phase difference for each of the different cell sizes in Figure 5.1. While it is understood that using a statistical probability of 99% represents very high bit error rates, the focus of this analysis is to illustrate the trade-offs that exist between the RMS voltage, operational temperatures and phase difference on the clocking electrodes for QCA circuits. Future work should consider higher probabilities, as well as methods of error correction in QCA devices. All cell parameters used are consistent with the previous simulations performed in this thesis.

Figure 5.1 shows that there exists trade-offs between the RMS voltage, operational temperatures and maximum phase difference of the clocking electrodes. While increasing cell size can significantly reduce the V_{rms} and number of clocking phases required for correct operation, it will come at the expense of room temperature operation. From Figure 5.1, to operate at room temperature, an RMS voltage of over 20 V is required while at least 100 clocking phases are necessary to ensure a statistical probability for correct operation remain at 99%

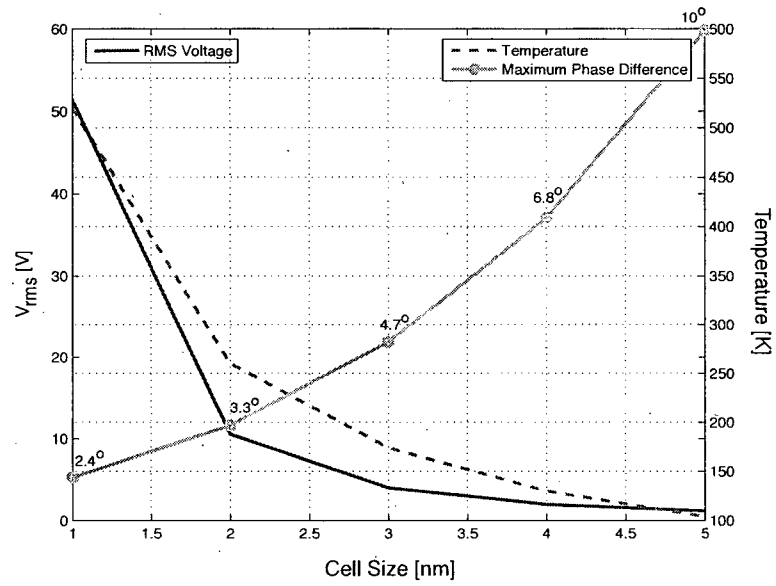


Figure 5.1: Required V_{rms} , maximum operational temperature, and maximum allowable phase shift vs. cell size to ensure a statistical probability of success of 99% for a majority gate. Trade-offs that exist between V_{rms} , the operational temperature and phase difference can be seen clearly in this figure.

Chapter 6

Random Phase Shifts on the Clock

As mentioned in Section 2.1.4, the clock signals act to pump information throughout the circuit via the successive latching and unlatching of cells connected to the different phases of the underlying clocking network. However, random phase shifts in the applied sinusoids can occur due to fabrication imperfections or uneven path lengths in the QCA circuit, and cause the circuit to malfunction or experience unexpected delays. The robustness of QCA circuits against such defects is examined in this chapter.

6.1 Zone Clocking

To simplify the simulations, a zone clocking scheme used by current QCA design tools is employed where all cells are grouped into one of four available clocking zones as depicted in Figure 6.1. Each cell in a particular clocking zone is connected to one of the four available phases in the QCA clock such that the transitioning from an ACTIVE state to a NULL state of each cell is synchronized with the changing clock signal.

When the clock value is low, the cells in that clocking zone will become latched (*i.e.*, switch to an ACTIVE state) and hold their value until the clock is relaxed (or *unlatched*), at which point the cell will enter the NULL state and remain so until the clock returns to its low value once again. An example of a binary wire using zone clocking is shown in Figure 6.2.

Notice that only one clocking zone in Figure 6.2 is latched while the others either remain or move into a relaxed state. As one clocking zone switches from a latched to a relaxed state, the next clocking zone latches and propagates the signal forward. The behaviour of the zone clocking scheme used here emulates the behaviour of the electrode clocking discussed earlier in this work, and hence provides a reasonable simplification for the purposes of this discussion. The size of the clocking zones is proportional to the separation between clocking electrodes.

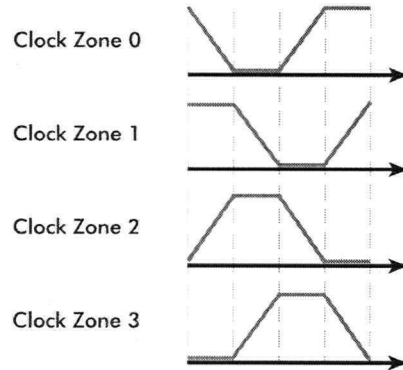


Figure 6.1: Zone Clocking. The four phases of the QCA clock are shown where each clocking zone is separated by a phase of 90° .

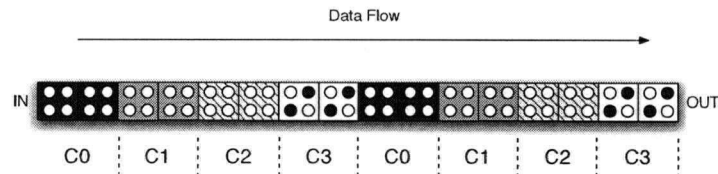


Figure 6.2: Binary wire using Zone Clocking. The four clocking zones are labelled C0, C1, C2 and C3 and are each represented with a different shade of gray. Here, clocking zone C3 is latching while the other three are relaxed.

6.2 Method of Simulation

Simulations on several QCA building blocks, shown in Figures 6.3-6.5, were conducted to study the impact of random phase shifts on the different clocking zones of the QCA clocking network. The steps for these simulations are described below:

1. For each of the simulated layouts in Figures 6.3-6.5, simulation results are generated without introducing any phase shifts to the four available clocking zones. These results were used as a reference for future simulations.
2. A set of 500 batch simulations is executed using a random variable, X , to represent the possible phase shift values as a fraction of $\pi/2$.

The random variable X is characterized by a Gaussian probability distribution function with mean value $\mu = i\frac{\pi}{2}$ and standard deviation σ , where i is the clocking zone number and $0 \leq i \leq 3$.

3. The percentage of successful circuits is recorded, where a successful circuit is any whose outputs matched those from Step 1.
4. Steps 2 and 3 are repeated for increasing values of σ .

Here, the interval $\sigma \in \{0, \pi/4\}$ was chosen with increments of $\pi/40$. σ values larger than $\pi/4$ would create phase shifts that are quite unlikely in reality and hence, are not considered in this study.

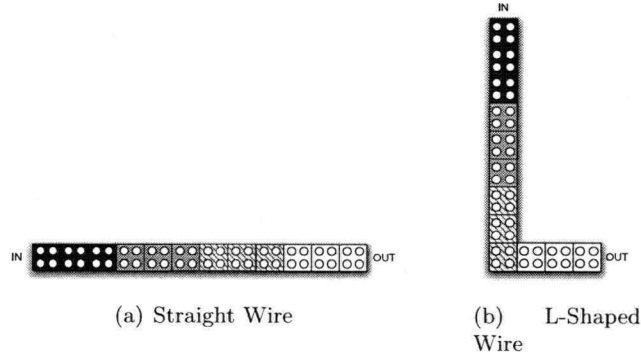


Figure 6.3: Simulated QCA Building blocks: (a) Straight Wire (b) L-Shaped Wire.

6.3 Simulation Parameters

Simulations were conducted using both the bistable (time independent) and coherence vector (time dependent) simulation engines available in QCADesigner [16, 18]. Cell sizes of 2 nm were used throughout with ϵ_r selected to be 1. A full summary of parameters used can be seen in Table 6.1.

The Clock High and Low energy values for both engines were determined by running 500 batch simulations on each circuit for the worst-case scenario ($\sigma = \pi/4$), and then plotting the number of successes versus the different Clock High and Low values as shown in Figures 6.6 and 6.8. The average number of successes for each Clock High and Low value over the number of devices was calculated (Figures 6.7 and 6.9) and then used to determine

	Bistable Engine	Coherence Vector
Temperature	N/A	0 K
Relaxation Time	N/A	1.11 e-16 s
Time Step	N/A	1.11e-18 s
Duration	N/A	1.11 e-12 s
Clock High	7.473e-20 J	7.473e-20 J
Clock Low	1.179e-20 J	1.179e-20 J
Clock Shift	0 J	0 J
Clock Amplitude Factor	2	2
Radius of Effect	200 nm	200 nm
Relative Permittivity	1.0	1.0
Layer Separation	1.15 nm	1.15 nm
Algorithm	N/A	Euler
Randomize Cells	Yes	Yes
Animate Simulation	No	No
Number of Samples	12800	N/A
Convergence Tolerance	0.001	N/A
max Iterations per sample	100	N/A

Table 6.1: Simulation Parameters

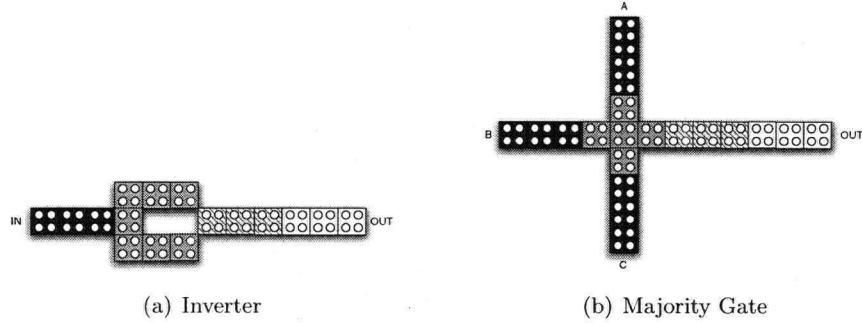


Figure 6.4: Simulated QCA Building blocks: (a) Inverter (b) Majority Gate.

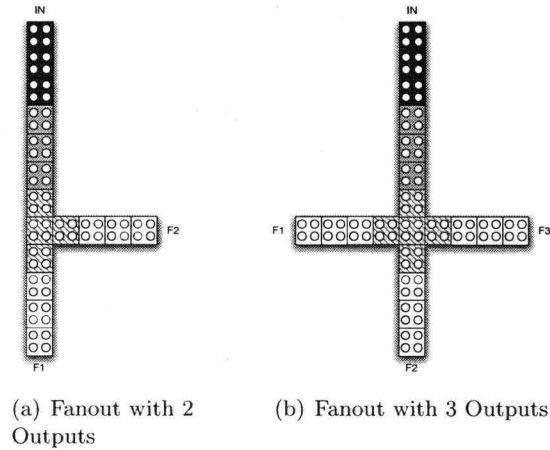
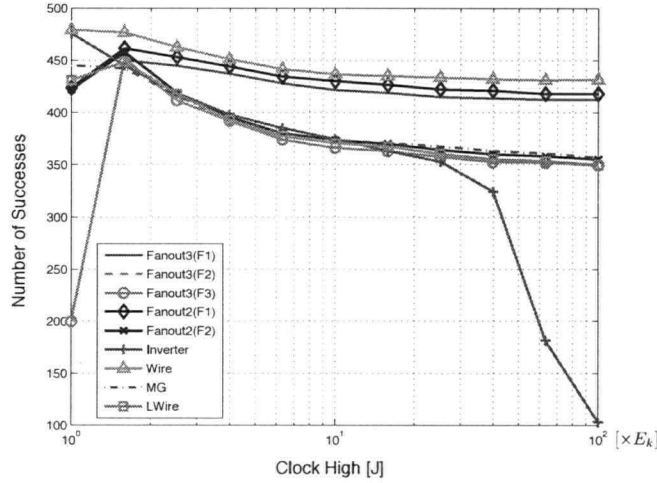


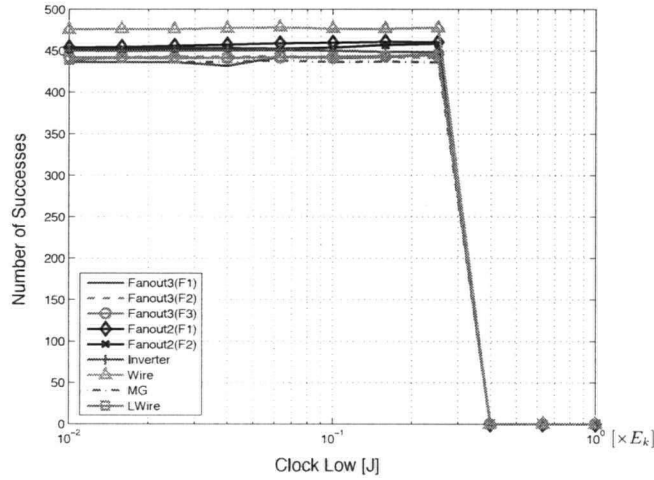
Figure 6.5: Simulated QCA Building blocks: (a) Fanout 2 (b) Fanout 3.

the optimal values for both simulation engines. The relaxation time, time step, and simulation time for the coherence vector simulation engine were selected to ensure that the solver converged, while the radius of effect was chosen large enough to encapsulate the entire circuit. All other parameters were kept at their default values.

From Figures 6.6-6.9, it can be seen that the simulated QCA building blocks behave similarly under both the bistable and coherence vector simulation engines with respect to the various Clock High and Low values with the exception that the bistable simulation engine produces higher success



(a) Number of Successes vs Clock High



(b) Number of Successes vs Clock Low

Figure 6.6: Number of successes of each considered QCA building block vs. the Clock High and Low values using the Bistable simulation engine.

rates. Figures 6.6(a) and 6.8(a) show that the optimal Clock High value lies at around $1.585E_k$ J for both simulation engines since the largest number of

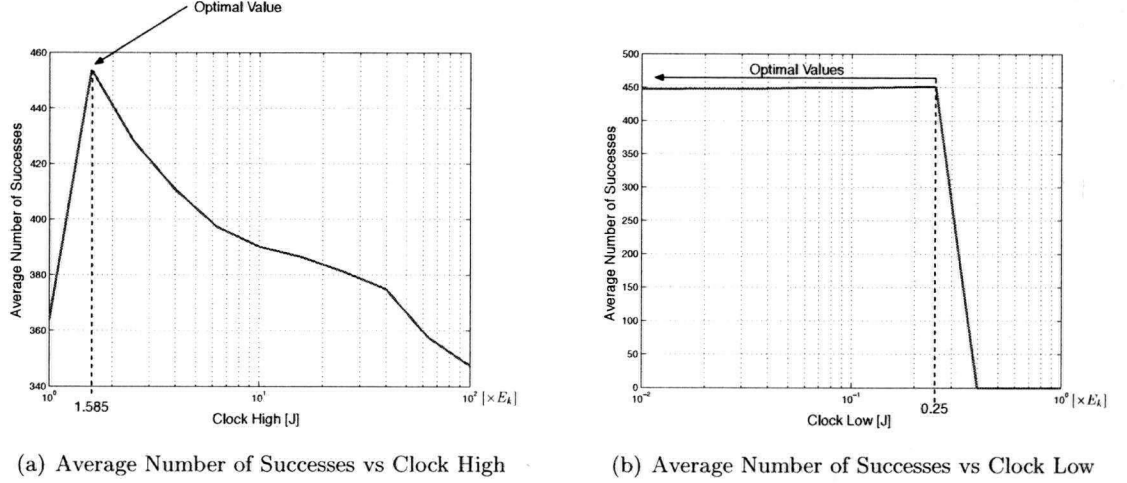
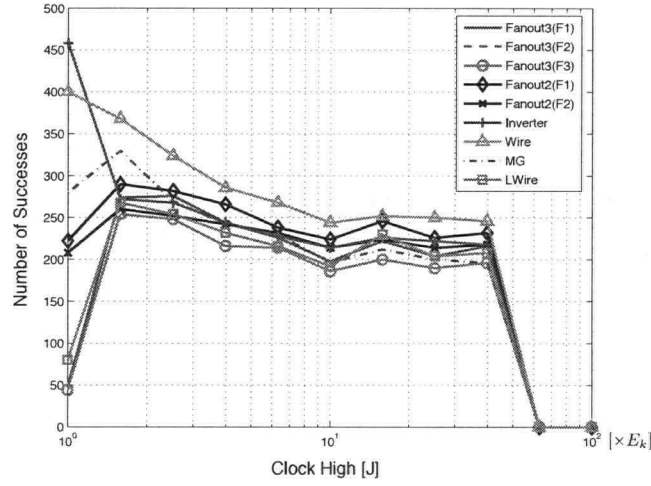


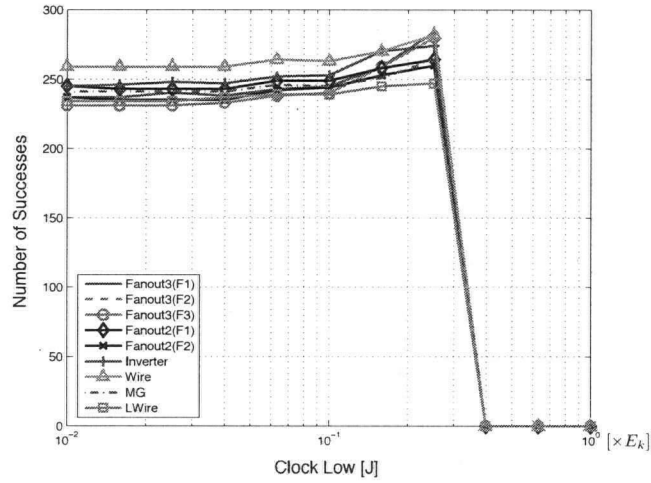
Figure 6.7: Average Number of successes for the considered QCA building block vs. the Clock High and Low values using the Bistable simulation engine. A Clock High value of $1.585E_k$ is desired while any value smaller than $0.25E_k$ provides an optimal value for the Clock Low.

successes occur at this Clock High value. Values smaller than $1.585E_k$ J may not allow a cell to fully unlatch - allowing it to perturb neighbouring cells in spite of its “relaxed” state. Ideally, large Clock High values are desired because as the Clock High value approaches infinity, the cells in that clocking zone will have $P = 0$. However, once random phase shifts are introduced into the clock, a clocking zone may enter a relaxed state before the next one has the opportunity to fully latch - creating a gap in the flow of information. In such cases, it is helpful to keep a Clock High value slightly lower such that it retains some residual polarization that can be used to perturb its neighbouring cells.

Figures 6.6(b) and 6.8(b) show that for a QCA circuit to begin functioning correctly, the Clock Low value must be smaller than $0.25E_k$ J. Larger values will not allow the cells to fully latch and hence the circuit will be unable to properly propagate the signal forward.



(a) Number of Successes vs Clock High



(b) Number of Successes vs Clock Low

Figure 6.8: Number of successes of each considered QCA building block vs the Clock High and Low values using the Coherence Vector simulation engine.

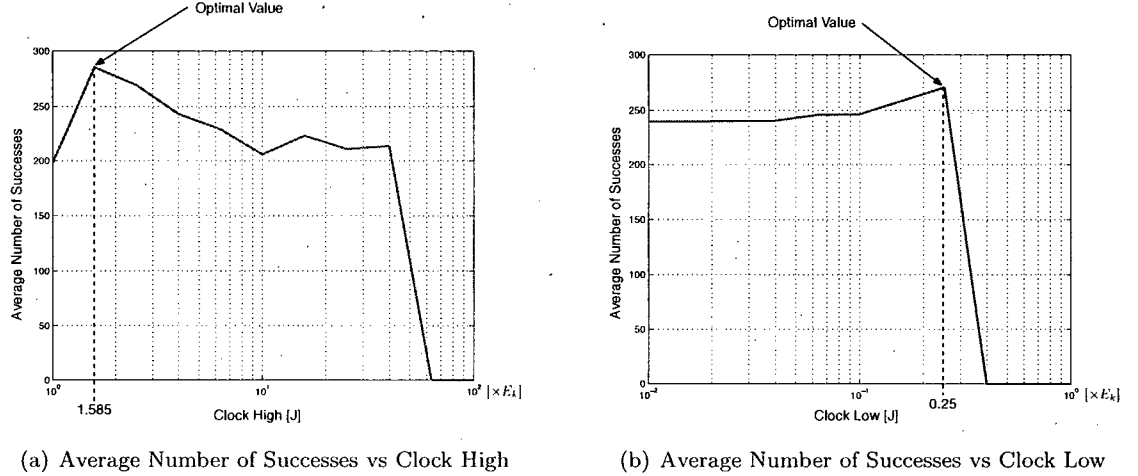


Figure 6.9: Average Number of successes for the considered QCA building block vs. the Clock High and Low values using the Coherence Vector simulation engine. A Clock High value of $1.585E_k$ is desired while $0.25E_k$ provides a good value for the Clock Low.

6.4 Fault Analysis

Faults due to random phase shifts in the clock can manifest themselves in one of two ways. They can result in either an unwanted delay or inversion at the primary outputs. The delays occur because the clocking zone to which the output is connected latches out of sequence, propagating the information either sooner or later than is expected. These delays can often be masked at the output if an unwanted inversion were to occur at the same time and cause us to incorrectly identify a faulty circuit as functional. Thus, it becomes critical that the input pattern be selected appropriately such that no such “false positives” occur. Here, the test sequence $\{0, 0, 1, 1, 0, 1, 0, 1\}$ is selected for all QCA building blocks featuring a single input, and $\{000, 100, 110, 010, 011, 001, 101, 111\}$ for the majority gate. These test sequences ensure that there exists no input dependency on the functionality of the primary outputs.

The unwanted inversions are slightly less intuitive. Consider the fanout circuit shown in Figure 6.10(a). In this figure, the signal has already propagated to the cells in clocking zone C1. Here, we expect C2 to move into

a latching state and propagate the signal forward. However, if phase shifts in clocking zones C2 and C3 are significant enough, then it is possible that the cells in C3 will latch before those in C2. If this occurs, then the cells in C3 will take on the opposite polarity of those in C1 due to the 45° angle that exists between their cells as shown by the NOT gates in Figure 6.10(b). Output F2 is not affected by this phase shift since it is lined up directly with the input. The same analysis can be applied to the Fanout2 building block as well.

If the Clock High value is selected appropriately ($\approx 1.585E_k$), then there will exist some residual polarization in the cells in C2 which may be sufficient enough to perturb the cells in clocking zone C3 and overcome the inversion. However for this to occur in either of the Fanout building blocks, the residual polarization left in the cells in C2 would have to be large enough to overcome the positive feedback that occurs between the outputs as shown in Figure 6.10(c). Here, after output Fanout3(F2) is latched, it interacts with both Fanout3(F1) and Fanout3(F3) and helps them remain in their current state and vice-versa. Similarly, outputs Fanout3(F1) and Fanout3(F3) will interact with one another helping each other to maintain their current states. Such is not the case, however, for the L-shaped wire. The LWire building block does not have any other outputs with which to interact and therefore, may be able to recover its correct output without any corruption, providing that there exists enough residual polarization in the cells in clocking zone C2.

The majority gate behaves similarly to the Fanout3 building block. Consider the majority gate shown in Figure 6.11(a). Here, the signal has propagated to the cells in clocking zone C0. Assume that the variations in the clock phase have caused C2 to latch before C1. As a result, inputs A and C will have an inverting effect on the output due to the 45° angle that separates them, while input B will attempt to directly influence the output. Figures 6.11(b) and 6.11(c) outline the two possible scenarios that need to be considered under these circumstances. The first is if inputs A and C are logically opposite. If such is the case then the output will simply be equal to input B and the inverting error that occurs due to inputs A and C goes unnoticed as shown in Figure 6.11(b). The second scenario occurs when both inputs A and C are logically equivalent. Under these circumstances, the inverting presence of these two inputs cannot be overcome and the output will bear the incorrect result as shown in Figure 6.11(c).

Another example of unwanted inversion can occur in the case of the inverter. Consider Figure 6.12(a). Here, the cells in clocking zone C0 are holding the signal to be propagated through the inverter. If the phase shifts

are such that the final clocking zone latches before C1 and C2, then the signal will propagate directly from the cells in C0 right to the output without undergoing any inversion as shown in Figure 6.12(b). Essentially, under this scenario, the inverter acts like a wire.

It is important to note that these circuits are simulated in a noise-less environment, *i.e.*, nothing in the circuit environment has the ability to influence a given cell other than its neighbours. All simulations are run at a temperature of 0 K in order to remove the influence of thermal noise.

6.5 Simulation Results

Figures 6.13 and 6.14 plot the simulation results for each of the layouts using the bistable engine and the coherence vector, respectively. In spite of the phase variations, the layouts remain robust even at high process variances in the clock for both simulation engines. For the bistable simulation engine, Figure 6.13 shows that circuits experiencing phase shifts in their clocking distribution network with standard deviations of up to 15% of $\pi/2$ can still operate at a 95% success rate. Similarly, from Figure 6.14, QCA circuits using the coherence vector simulation engine can operate at a 90% success rate while withstanding phase shifts with standard deviations of 10% of $\pi/2$ in its clocking distribution network. The non-monotonic behaviour of the results shown in Figures 6.13 and 6.14 are likely a result of not simulating a large enough sample size. Future work should look to expand the number of batch simulations performed.

From Figures 6.13 and 6.14, the outputs of the considered QCA building blocks segregate themselves into one of three groups. The first group of outputs are those that resemble a straight wire, *i.e.*, represent a straight path from the input to its output. The Wire, Fanout2(F1) and Fanout3(F2) all fall into this group of outputs. This group sees the highest success rate of any other group because the variations in clock phase can only cause delay at these outputs as mentioned in Section 6.4, and are not affected by any unwanted inversion.

The second group of outputs are those belonging to either Fanout2 or Fanout3 that do not see a straight path from the input to its output, *i.e.*, there exists a 90° bend (“kink”) between the input and output. It is clear from Figures 6.13 and 6.14 that the outputs that belong to this group - Fanout2(F2), Fanout3(F1) and Fanout3(F2) - produce the worst success rate of any group due to the potential of unwanted inversion at the outputs as discussed in the previous section.

The third group consists of the LWire, MG, and Inverter building blocks. For reasons described in Section 6.4, these building blocks have success rates that lie in between the other two mentioned groups.

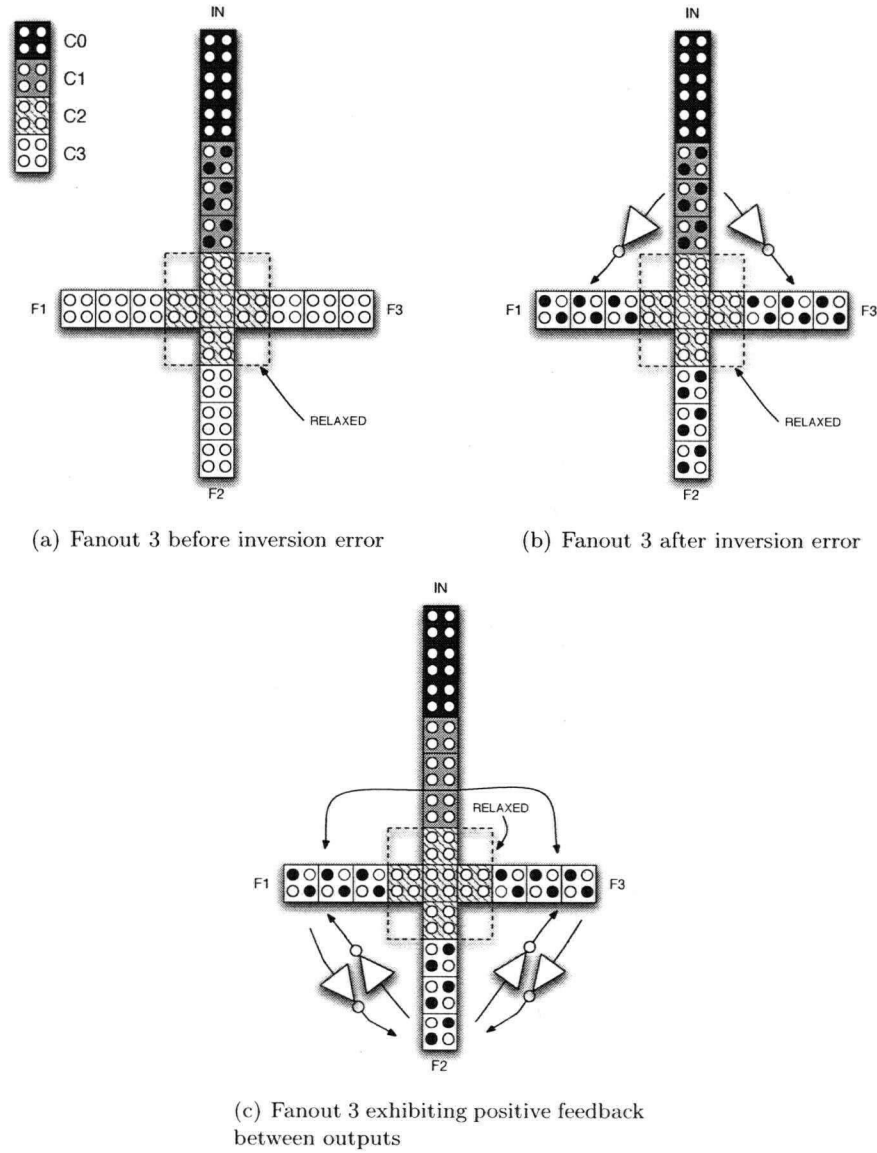
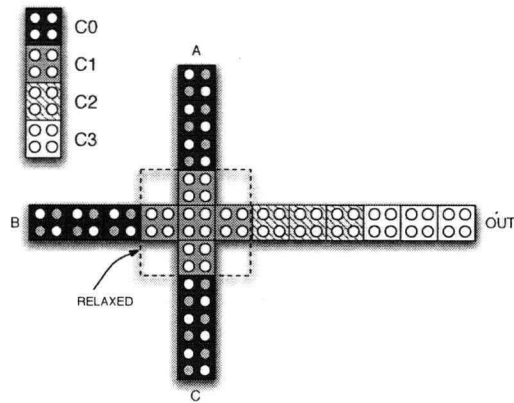
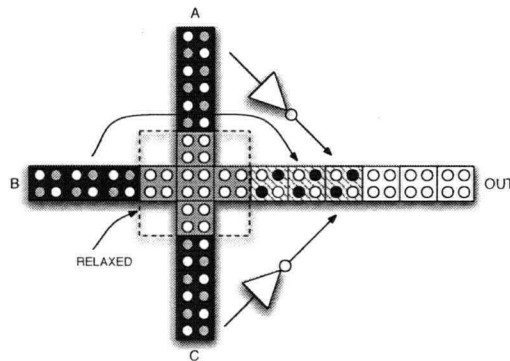


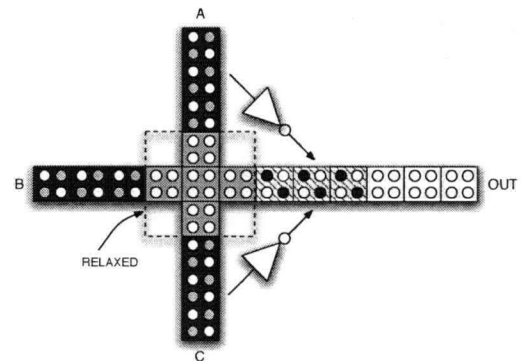
Figure 6.10: Inversion error in the Fanout3 circuit. If clocking zone C3 latches before C2, then two of the outputs will experience unwanted inversion (F1, F3). The different clocking zones are labelled in the top-left hand corner for reference.



(a) Majority Gate before inversion error



(b) Majority Gate recovering from inversion error



(c) Majority Gate failing due to inversion error

Figure 6.11: Inversion error in the majority gate circuit. If clocking zone C3 latches before C2, then the output may see the logical inverse of what it is supposed to. The different clocking zones are labelled in the top-left hand corner for reference.

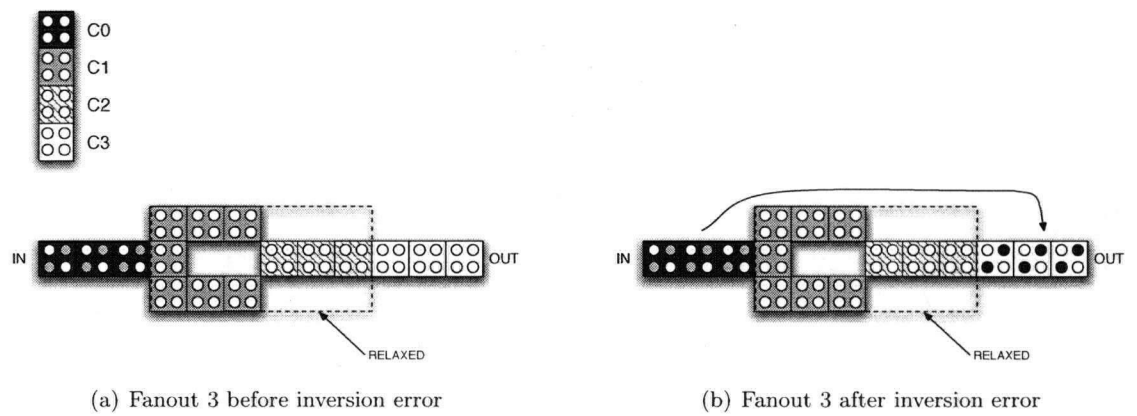


Figure 6.12: Inversion error in the inverter circuit. If clocking zone C3 latches before C1 and C2, then the output will simply take on the value of the input, effectively replicating the behaviour of a straight wire. The different clocking zones are labelled in the top-left hand corner for reference.

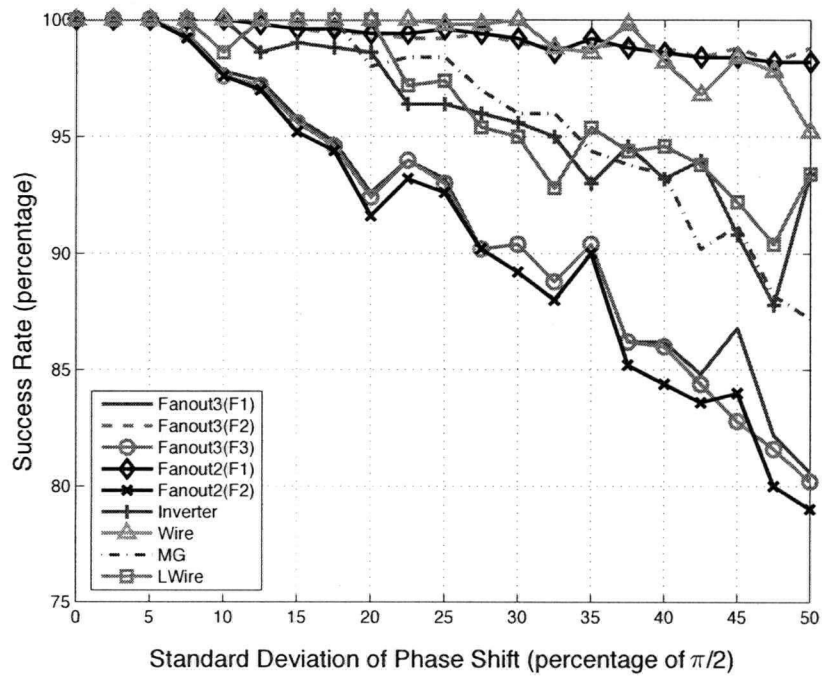


Figure 6.13: Success Rate vs Standard Deviation of the phase shift for the Bistable Simulation Engine.

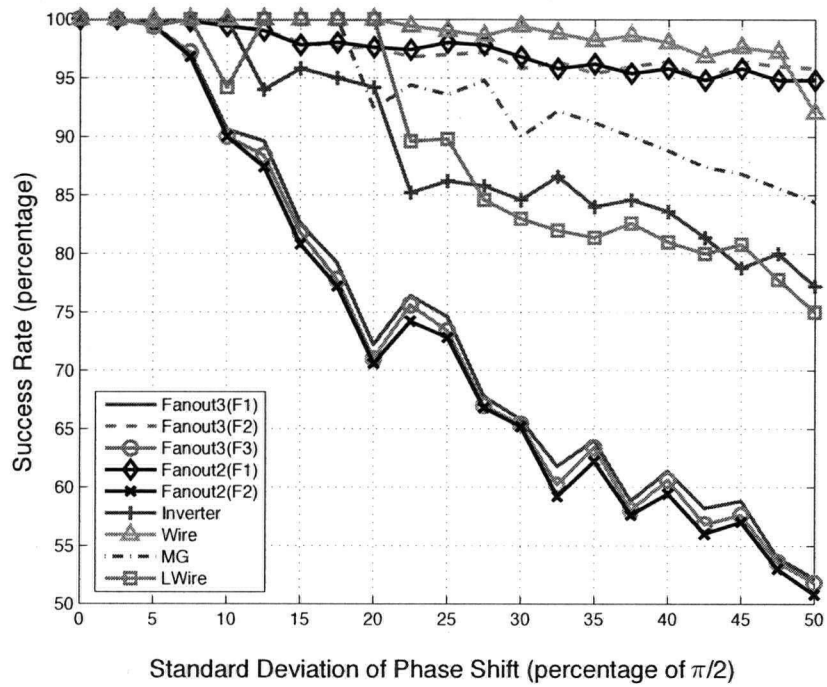


Figure 6.14: Success Rate vs Standard Deviation of the phase shift for the Coherence Vector Simulation Engine.

Chapter 7

Conclusions

Analytical expressions were derived for the energies associated with the ACTIVE, NULL and X states of a QCA cell. Furthermore, limitations were established on the applied potential and phase of the clocking electrodes to ensure proper functionality of fundamental building blocks in a QCA circuit. It is understood that arbitrary molecular geometries and neutralizing charge distributions cannot be realized using real systems. This work provides a good comparison between molecular systems that can be generalized to this modelled geometry. The limits presented in this thesis will serve to aid in the selection of molecular structures. In addition, the selection of appropriate molecular structures and design of clocking electrodes will reduce the power consumption of the underlying clocking distribution network. It was also shown that there exists a relationship between the required switching potential and cell size. As the cell size is decreased, the minimum potential required to switch a cell from an ACTIVE to a NULL state is increased. These results express the trade-offs between switching voltage, operating temperature and maximum phase shift on the clocking electrodes. The switching voltage and number of clocking phases increase significantly as cell sizes are decreased in an attempt to increase the operating temperature of these devices. Such high switching voltages will result in significant power dissipation in the clocking network. It is concluded that irrespective of the fact that individual devices can operate with little power consumption, the clocking infrastructure required to support computation will most likely consume most of the power.

Lastly, the effect of random phase shifts on the underlying clocking network was investigated. Simulations were run on a set of universal QCA building blocks, *i.e.*, they can be used to implement arbitrary QCA circuits, and were repeated using both the bistable and coherence vector simulation engines in QCADesigner. All devices were fairly robust against variations in the clock signal phases, with success rates of over 90% for phase shifts with standard deviations of up to 10% of $\pi/2$. We found that the success rate of a given output is highly layout-dependant. Outputs resembling a straight wire displayed more robustness to the phase variations than did

those featuring kinks in their wire. As a result, QCA building blocks can be segregated into distinct classes depending on the number of kinks and outputs that they contain making it easier to pre-determine sensitive areas in a circuit due to phase variations in the clock. These results should help in developing fabrication specifications for QCA clocking networks.

Future work in this area should extend this work to consider the dependency of switching potential, operational temperature, and phase difference of the clocking electrodes on other circuit parameters such as the distance between the ground plane and electrodes, η , the cell elevation, β , and the relative permittivity between the electrodes and molecules, ϵ_{r2} . A higher statistical probability to measure the success rate of QCA circuits should also be considered along with possible methods of error correction. Lastly, the phase shift analysis should be extended to include the large number of phases found to be necessary in this work.

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