Computational Modeling of Rapid Thermal Processing in a Chemical Vapor Deposition Reactor for Catalytic Growth of Carbon Nanotubes

by

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Scalable manufacturing of uniform carbon nanotube (CNT) structures requires careful control of temperature profiles and gas flow rates inside complex chemical reactors. In this work, Ansys[®] CFX, Release 2021 R2 is used to model the spatiotemporal evolution of temperatures inside a custom-designed multizone chemical vapor deposition (CVD) reactor with rapid thermal processing (RTP) capabilities. Heat is primarily generated by a set of twelve infrared (IR) lamps distributed both above and below the quartz tube in the reaction zones. Radiation is modeled using the Monte Carlo radiation model in Ansys CFX. A catalyst-coated substrate is placed on a silicon wafer held in the middle of the reactor using quartz rods. A thermocouple located beneath the wafer is modeled as a composite, wherein an area-weighted average of all the components was used to determine bulk material properties. A mesh convergence study consisting of three refinements was carried out to ensure proper mesh size. The model is then validated by comparing simulation results to experimental research relating the power supplied to the infrared lamps and the temperature rise dynamics measured by the thermocouple. Results show that the model adequately captures the behavior of the reactor, and can hence be used to accurately explain the influence of different boundary conditions on the spatial distribution of temperatures as well as the rate of heating of both the thermocouple and the catalyst. Accordingly, the model is powerful for the design of new wafer holder geometries and materials to precisely control the temperature distribution around the catalyst in order to achieve geometric and morphological uniformity in asgrown CNT forests.

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Preface

First, I would like to thank my advisor, Dr. Mostafa Bedewy, for all of his support and guidance throughout this project. Having a mentor who believed in me since I was an undergraduate and who helped me grow so much throughout graduate school is something I will always be grateful for. I would also like to thank my committee members, Dr. Shervin Sammak, Dr. Inanc Senocak, and Dr. Sangyeop Lee for their valuable insights.

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1.0 Introduction

1.1 Chemical Vapor Deposition (CVD) Process

The chemical vapor deposition (CVD) process generally refers to a process in which a chemical reaction of gaseous precursors takes place, forming a thin solid film on a given substrate material.¹ A precursor is a compound, which can be in the gas phase or on the substrate, that is a part of the chemical reaction that produces another compound, such as the one that forms on the substrate. These reactions can be initiated in several ways, most commonly by heat in the case of thermal CVD, or by high frequency radiation like UV in photo-assisted CVD. There is also catalytic CVD, which is often used to grow carbon nanotubes (CNTs).

1.2 Types of CVD Reactors

There are many types of CVD reactors and processes, such as metal-organic CVD (MOCVD) and plasma-enhanced CVD (PECVD). Most CVD processes are initiated thermally, using thermal radiation heating, radio-frequency (rf) induction of the substrate or holder, or direct resistance heating of the substrate or holder to name a few¹. Other processes, like PECVD, allow the reactions to take place at lower temperatures by using electrical energy instead of thermal energy to initiate reactions. Thermal CVD reactors are classified as either hot-wall or cold-wall. In a hot-wall reactor, the whole reactor is placed inside an oven. For the case of a tube reactor, the deposition zone is placed inside an oven¹. In this type of reactor, the substrate, reactor walls, and

gas are all at the same temperature. In a cold-wall reactor, the substrate heats the gas that flows over it¹. In this type of reactor, the reactor walls and gas are kept at a temperature lower than the substrate, which is sometimes ambient temperature. Figure 1 shows some common schematics of hot-wall and cold-wall tube reactors, commonly used for research applications.



Figure 1 Examples of cold-wall and hot-wall tube reactors¹, republished with permission of Royal Society of Chemistry, permission conveyed through Copyright Clearance Center, Inc.

1.3 Rapid Thermal Processing (RTP) in CVD

Another method of heating in thermal CVD reactors is rapid thermal processing (RTP). This is usually accomplished using transient lamp irradiation to heat a substrate or with a continuous heat source where the substrate would be moved in and out of the heated area. Figure 2 provides a schematic of a RTP reactor where a series of tungsten halogen infrared lamps are used to heat a silicon wafer through radiation². Figure 3 shows a schematic for a different type of RTP chamber, where light from a 200 kW arc lamp shines through a quartz window and heats the bottom of a silicon wafer uniformly³. There are no lamps on top, but instead this chamber has a reflective metal grid above the wafer called a showerhead where gas can be injected.

In CVD reactors, one benefit of using RTP is that multiple layers can be grown without removing the wafer from the chamber thus reducing the risk of contamination⁴. This requires the temperature to be rapidly adjusted for each layer. Because of this, temperature measurement and control when using RTP in CVD is extremely important and so is temperature uniformity. These reactors typically use thermocouples, which are either embedded into a silicon chip near substrate or located in the immediate vicinity of the substrate, such as directly under it. Some issues with this include the changing of the chip's absorptivity as the deposition takes place, and also the degradation of the thermocouple itself over time due to the rapid thermal cycling. Non-contact temperature measurement is one solution to these problems, such as *in situ* monitoring of a specific material property that is dependent on temperature. *In situ* measurement is also beneficial in studying other properties, such as the growth kinetics of vertically aligned carbon nanotubes $(VACNTs)^{5.6}$.



Figure 2 Schematic of the RTP reactor described in Logerais et al², reprinted with permission from Elsevier



Figure 3 Schematic of the RTP chamber described in Wacher and Seymour³, reprinted with permission from

Brian Seymour

1.4 Importance CVD Reactors to Grow CNT

One of the applications of CVD is the growth of carbon nanotubes (CNTs), as discussed previously. Carbon nanotubes are an allotrope of carbon, made of cylindrical carbon molecule structures with dimensions in nanometers.⁵ It is often desirable to grow these nanotubes in forests, where many individual CNTs grow vertically aligned on a substrate. Figure 4 shows a scanning electron microscopy (SEM) image of a typical CNT forest showing good alignment and high density^{5,7}, which are very good qualities for a CNT forest to have. This figure also shows, in the upper right corner, the actual CNT forest as it appears when taken out of the reactor. When CNTs are grown this way, they possess many desirable qualities such as high surface area, good electrical conductivity, and high carbon purity⁸. These qualities make the CNTs extremely valuable in several industries for use with products like stretchable conductors, fuel cells, and sensing applications⁸ to name a few. CNTs also have many uses in the biomedical industry, shown in Figure 5⁹, and in the aerospace and electronics industries.



Figure 4 SEM image of a CNT forest⁷, reprinted with permission, copyright 2021 Americal Chemical Society



Figure 5 CNT applications in the biomedical industry⁹, reprinted with permission from Elsevier

CVD is the most viable method of CNT growth on an industrial scale, but it does require a high degree of temperature and pressure control. Spatiotemporal maps of temperature are also important to track CNT growth, and one way to do this is through modeling and simulation. Modeling a CVD reactor that is used for CNT growth would allow researchers to obtain a spatiotemporal map of the temperatures on the silicon wafer. This temperature map would allow researchers to develop a better understanding of the nonuniformities that occur in CNT forests. For example, Figure 6 shows two extreme cases of nonuniformities that can occur in CNT forests, the forest has a hole in the center (top) or the forest only grows in the center (bottom).



Figure 6 Nonuniformities in CNT forests

1.5 Description of NanoProduct Lab's RTP CVD Reactor

Figure 7 presents a schematic of the NanoProduct Lab's custom designed RTP CVD reactor used for the catalytic growth of CNTs^{10,11}. The gases are preheated in a resistive furnace and these gases are sent into the RTP furnace via the helical injector. The flow of these gases is controlled using mass flow controllers. The RTP furnace consists of 12 infrared (IR) lamps, six on the top and six on the bottom. These lamps create a multizone IR heater with three zones, each zone consisting of two lamps on the top and two lamps on the bottom. The three zones can be controlled and the top and bottom lamps can also be independently controlled. The growth of the CNTs takes place in this RTP furnace. The temperature in this furnace is monitored by three thermocouples embedded in a quartz arm that supports the catalyst wafer. They are staggered at about one inch, where the centermost thermocouple is located under the center of the catalyst wafer. These thermocouples are connected to a digital temperature reader, and the signals are used

in a closed-loop control system which determines the lamp powers in each zone. The use of these IR lamps allows the furnace to be well lit, thus allowing the CNT growth to be monitored in real time through a viewing port using a high magnification camera. Using image processing, the growth rates can be measured from the time evolution of forest height.



Figure 7 Schematic of NanoProduct Lab's RTP CVD reactor¹¹, reprinted with permission, copyright 2019 American Chemical Society

1.6 Importance of Modeling Custom CVD Reactors

As discussed previously, creating spatiotemporal maps of temperature when using CVD for CNT growth is extremely valuable. There are several ways to do this, but using a computational fluid dynamics (CFD) model presents many benefits. First, this type of modeling allows for both the fluid flow of the gases and the flow of the radiative heat to be tracked simultaneously. This also allows the user full control over the creation of the solid model, which is important in the case of a unique, custom designed reactor like the one used in the NanoProduct Lab. When using a CFD model of a reactor, the user can also change parameters such as the type of gases or substrate and examine the results before having to change them in the reactor. This allows for the user to examine

the benefits and drawbacks of the experiment before conducting it and can be a way to save not only resources but time.

As mentioned earlier, another issue in RTP CVD is substrate temperature measurement and control and temperature uniformity. This is particularly difficult due to several factors specific to the reactor in Figure 7. First, the radiative properties (absorptivity, emissivity, reflectivity) of the thermocouple and the substrate are different, and the thermocouples are embedded in the quartz arm and not actually touching the sample. This means that the signals from the thermocouples that are sent back to the closed-loop control system are not the actual substrate temperature. A CFD model of the RTP furnace would allow the user to examine the thermocouple temperature in comparison with the temperature of the actual substrate, and then understand the difference between the wafer/substrate temperature profile and the thermocouple temperature readings.

1.7 Challenge of Modeling IR Reactors

Creating a computational fluid dynamics (CFD) model of an IR reactor presents several challenges. In general, determining a satisfactory time stepping scheme and mesh is always a factor in any CFD project, and these were especially important in this case. A model that includes radiative heat transfer adds much more complexity, and thus many more factors to work out. Historically, the Monte Carlo radiation model is most frequently used in simulations involving IR reactors, and this is the radiation method used here. Another important consideration in CFD modeling is how to model turbulence, which in this case involved researching and selecting the correct turbulence model in Ansys CFX. Because of the radiation-driven nature of the simulations, the choice of turbulence model was prioritized by wall time as opposed to resolution. As a result

the two-equation, shear stress transformation (SST), turbulence model was chosen. Furthermore, convective heat flux was determined to be insignificant in the IR chamber compared to the magnitude of radiative heat flux. This also justifies the decision to set the fluid domains to non-buoyant. Another set of challenges when creating a CFD model of a CVD reactor comes with the small measurements of the geometry. For example, the catalyst wafer is very small and thus requires highly refined and dense mesh with a large number of elements to capture the temperature distribution, and a larger number of elements in a CFD model greatly increases computation time. Some parts of the model can be simplified to reduce the number of elements and computation time, such as omitting thermally irrelevant parts of the geometry, which will be discussed in detail in later sections.

1.8 Description of Experiments

Recipes are programmed for use in the custom designed RTP CVD reactor. These recipes were designed to examine how the lamp power in each zone effects the steady state temperature of the preheater and each RTP furnace zone and the time it takes to reach steady state temperature. Before each recipe starts, the preheater and all RTP furnace zones are at ambient temperature. Then, the IR lamps are turned on and warmed up for one minute, and the power to each zone is manually set from 0% to 65%. Once the desired steady state temperature is achieved in all zones, the recipe is ended and the reactor is allowed to cool down before starting the next recipe. Helium flows in at a rate of 1700 SCCM (standard cubic centimeters per minute), and the sample is an alumina-supported iron catalyst placed on a silicon chip. This sample sits on top of a two-inch

fused silica wafer that is positioned on the quartz arm and is kept inside the reactor so that changes to the position of the sample do not create inconsistencies.

1.9 Review of Previous Work

1.9.1 Modeling and Simulation of IR Reactors

In recent years, there have been many others that have explored modeling and simulation of IR reactors, and modeling the IR lamps seems to be one of the biggest challenges. Logerais et al^{2,12} uses the Monte Carlo method in a 3D CFD model of an IR reactor to calculate radiative heat transfer from the lamps, similar to this work. However, the geometry and thermal boundary conditions of the lamps differ from this model. Logerais et al^{2,12} models the quartz bulb, tungsten filament, and nitrogen inside the lamp. Then, temperatures specific to a certain lamp power percentage are applied to the tungsten filament modeled as a cylinder in the center of the lamp. Jenkins et al¹³ models only the filament of the lamps. Turner and Ash¹⁴ model both the filament and the quartz bulb, but the filament is treated as the primary source of heat generation. Jadachowski et al¹⁵ created a 1D model where the IR lamps are modeled as infinitely long opaque cylinders and uses the net radiation method to calculate the radiative heat flow in the IR zone. Yu et al¹⁶ showed that their quartz lamps could be modeled as a slat with the same temperature radiation source.

Modeling radiative heat transfer is also a heavily researched topic in recent years. In modeling radiative heat transfer in IR chambers, use of the Monte Carlo method is the most common^{2,12,14}. However, some other use different methods. For example, Wacher and Seymour³

use shape factor theory to calculate the radiative heat transfer in a rapid thermal processing system. Jenkins et al¹³ used the Discrete Ordinates (DO) model in Ansys Fluent, and Yu et al¹⁶ uses a finite volume method algorithm to capture the radiative heat transfer from quartz lamps in their system. Chao et al¹⁷ studies on the effect of lamp radius on thermal stresses that contribute to wafer temperature nonuniformity focusing on edge effects. They treat the problem as a 1D plane stress model using a fully implicit finite difference method. The effects of radiative heat transfer are quantified using the law of radiative heat transfer to obtain view factors between the lamps and the wafer, where the tungsten-halogen lamps are modeled as flat black body radiation sources.

1.9.2 What is New and Unique about this Work

This work is unique and presents new methods that have not been used in combination previously. The IR lamps are modeled as hexagons instead of cylinders, as this proved to decrease the mesh size and the computational run time without changing the temperature results. The lamps are also modeled as "voids", meaning that the actual lamps are not present in the model. Instead, lamp-shaped holes are made in the fluid inside the IR chamber and the thermal boundary conditions are applied to the outer fluid surface that would be in contact with the lamps if they were present. A relation between the lamp net radiative flux and lamp temperature is used to create simulations for a specific lamp power, which has not been done previously. This work also measures both thermocouple and wafer temperature, while previous works tend to focus on just one of these.

2.0 Methods

2.1 Material Properties

One of the first steps in setting up a simulation in Ansys[®] CFX, Release 2021 R2, is to define the material properties to be used in each domain. Several of these materials were already present in the Ansys material library, such as Air at STP and He at STP, however the rest of the materials used in the model needed to be defined by the user. The material properties for gold, silicon, and fused silica (quartz) are well documented and were easily obtained from various sources¹⁸. For example, the density, specific heat, and thermal conductivity values at 300 K were obtained from Fundamentals of Heat and Mass Transfer¹⁸. However, defining the material properties for the thermocouple (TC) was more complex and will be discussed in detail in later sections. Table 1 shows a table of all the material properties that necessary to define each material in Ansys[®] CFX, Release 2021 R2.

Table 1 Material properties

Material	Fused Silica	Gold	Silicon	Air at STP	He at STP	TC
State	solid	solid	solid	gas	gas	solid
Molar Mass	60.08 g/mol	196.97 kg/kmol	28.0855 kg/kmol	28.96 kg/kmol	4.00 kg/kmol	51.378136 kg/kmol
Density	2220 kg/m ³	19300 kg/m ³	2330 kg/m ³	1.284 kg/m ³	0.179 kg/m ³	6576.112416 kg/m ³
Specific Heat Capacity	745 J/kgK	129 J/kgK	712 J/kgK	1.0038e+3 J/kgK, constant pressure	5240 J/kgK, constant pressure	618.9632 J/kgK
Reference State	Temp: 300 K	Temp: 300 K	Temp: 300 K	Temp: 0C, Pressure: 1 atm	Temp: 0C, Pressure: 1 atm	Temp: 25 C
Reference Specific Enthalpy	0 J/kg	0 J/kg	0 J/kg	0 J/kg	-1.2982658e+5 J/kg	0 J/kg
Reference Specific Entropy	0 J/kgK	0 J/kgK	0 J/kgK	0 J/kgK	3.1034571e+4 J/kg/K	0 J/kgK
Thermal	1.38	317	148	2.428e-2	1415e-4	8.66936
Conductivity	W/mK	W/mK	W/mK	W/mK	W/mK	W/mK
Dynamic Viscosity	n/a	n/a	n/a	1.725e-5 kg/ms	18.6e-6 kg/ms	n/a
Refractive Index	1.4585	1.16901	3.9766	1	1	1
Absorption Coefficient	0.1 1/m	7.0051e+7 1/m	646050 1/m	0.01 1/m 1 1/m		1 1/m
Scattering Coefficient	0 1/m	0.5 1/m	0 1/m	0 1/m	0 1/m	0 1/m
Thermal Expansivity	n/a	n/a	n/a	0.00366 1/K	0.00366 1/K	n/a

2.2 Governing Equations

Ansys CFX solves the unsteady Navier-Stokes equations in their conservation form, according to the Ansys CFX-Solver Theory Guide¹⁹. These equations include the transport

equations; continuity (2.1), momentum (2.2) and the stress tensor τ and its relation to strain rate (2.3), and total energy (2.4) and the total enthalpy h_{tot} and its relation to static enthalpy h(T, p) (2.5).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}) = 0 \tag{2.1}$$

Where ρ is density and **U** is the vector of velocity ($U_{x,y,z}$).

$$\frac{\partial(\rho \boldsymbol{U})}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} \otimes \boldsymbol{U}) = -\nabla p + \nabla \cdot \tau + \boldsymbol{S}_{M}$$
(2.2)

Where p is static (thermodynamic) pressure, τ is shear stress (or sub-grid scale stress) molecular stress tensor, and S_M is the momentum source term.

$$\tau = \mu (\nabla \boldsymbol{U} + (\nabla \boldsymbol{U})^T - \frac{2}{3}\delta \nabla \cdot \boldsymbol{U}$$
(2.3)

Where μ is molecular (dynamic) viscosity, *T* is static (thermodynamic) pressure, and δ is the identity matrix or Kronecker Delta function.

$$\frac{\partial(\rho h_{tot})}{\partial t} - \frac{\partial p}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} h_{tot}) = \nabla \cdot (\lambda \nabla T) + \nabla \cdot (\boldsymbol{U} \cdot \tau) + \boldsymbol{U} \cdot \boldsymbol{S}_{\boldsymbol{M}} + \boldsymbol{S}_{\boldsymbol{E}}$$
(2.4)

Where h_{tot} is specific total enthalpy, λ is thermal conductivity, and S_E is the energy source term.

$$h_{tot} = h + \frac{1}{2} U^2 \tag{2.5}$$

Where h is specific static (thermodynamic) enthalpy.

2.3 Selecting a Radiation Model

The main objective of radiation modeling in Ansys CFX is to solve the radiation transport equation and obtain the source term for the energy equation (2.4) described previously. The spectral radiative transfer equation (RTE), according to the Ansys CFX-Solver Theory Guide¹⁹ is shown in (2.6).

$$\frac{dI_{\nu}(\boldsymbol{r},\boldsymbol{s})}{ds} = \left(-(K_{a\nu} + K_{s\nu})I_{\nu}(\boldsymbol{r},\boldsymbol{s}) + K_{a\nu}I_{b}(\nu,T) + \frac{K_{s\nu}}{4\pi}\int_{4\pi}dI_{\nu}(\boldsymbol{r},\boldsymbol{s}')\Phi(\boldsymbol{s}\cdot\boldsymbol{s}')d\Omega' + S\right)$$
(2.6)

Where I_v is spectral radiation intensity which depends on position r and direction s, r is the position vector, s is the direction vector, s is path length, v is frequency, K_a is the absorption coefficient, K_s is the scattering coefficient, I_b is Blackbody emission intensity, T is local absolute temperature, Φ is the in-scattering phase function, Ω is the solid angle, and S is the radiation energy source term or particle-radiation interactions.

Solving the RTE is very time consuming, thus Ansys CFX includes directional and spectral approximation models. The radiation models involving directional approximations are Rosseland, P1, Discrete Transfer, and Monte Carlo. Each of these models also contain spectral approximations, or spectral models.

The Rosseland model simplifies the RTE for optically thick media by introducing a new diffusion term which contains a strongly temperature dependent diffusion coefficient¹⁹. This model is typically recommended for optical thicknesses greater than five. It is also important to note that this approximation is not valid near walls, because this model assumes that radiant energy emitted from other areas in the domain do not have influence on the local transport because they are quickly absorbed²⁰. Thus, a boundary condition must be specified for wall treatment.

The P1 model simplifies the RTE by assuming that the radiation intensity is isotropic or direction independent at a given location in space¹⁹. At the walls, it is assumed that the radiation intensity coming into or going out of a wall are directionally independent, and a specific boundary condition is needed. The P1 model is typically recommended when the optical thickness is greater than one. When using this model, the diffuse fraction setting on walls is ignored, as this model

only allows for diffuse opaque walls. It also treats all open boundaries, such as inlets, as fully transparent meaning that they absorb all outgoing energy and incoming energy is calculated as a blackbody²⁰.

The Discrete Transfer model simplifies the RTE by assuming that the scattering is isotropic. This model is based on the discretization of the transfer equation along rays, and tracing the domain using multiple arrays leaving from boundary surfaces²⁰. This model is only valid for optically thin or transparent media.

Lastly, the Monte Carlo model assumes that the intensity is proportional to the differential angular flux of the photons, where one can consider the radiation field as a photon gas, and then the absorption coefficient is the probability per unit length that a photon is absorbed at a given frequency¹⁹. Similar to the way Discrete Transfer model traces rays, this model tracks photons through a domain.

In the very early stages of the project, the P1 radiation model was used, but shortly after it was determined to be unsatisfactory and it was decided that Monte Carlo would better suit this model. This is due to several factors. First, Monte Carlo can be used in both solid and fluid domains, and it was determined that radiation would need to be used in all domains, so this was the best option. Monte Carlo can also be used if the medium is optically thick or thin, while the P1 model should only be used if the medium is optically thick. Optically thick implies that the domain is opaque, meaning that the average photon cannot pass through the medium without absorption, and a fluid will absorb and then re-emit radiation that passes through it. Optically thin implies that the domain is transparent, and radiation only interacts with boundaries of the domain. Another benefit of the Monte Carlo model is that it can be used in both transparent or semi-transparent domains, and this model contains both. This thermal radiation model also includes both a surface

to surface and participating media transfer mode for all domains. As described in the Ansys CFX Solver Modeling Guide²¹, the surface to surface option ignores volumetric emission, absorption, and scattering even if these values are specified in the properties of the material assigned to the respective domain. The participating media transfer mode does the opposite, meaning that the domain material will emit, absorb, and/or scatter radiation. The surface to surface model is used in all fluid domains, the paddle, and the tube. This is because these are not the main subject of the simulations, therefore radiation should just pass through these domains. The participating media model is used in the wafer, solid box, and thermocouple domains, as these are the main focus of the simulation and it is important to see the effects of radiative heat transfer on these parts. The spectral model used in all domains is Gray, which assumes that all radiation quantities are nearly uniform. This means that radiation intensity is the same for all frequencies, and thus the dependency of the RTE on frequency is dropped.

When using the Monte Carlo model, it is also important to select an appropriate number of histories. This number of histories is used in the Monte Carlo statistics calculations¹⁹ and is divided into several groups. Then, histories are selected from each group and their physical interactions are tracked through the domain. Some of the physical interactions include emission, absorption, and reflection. Once the calculation is complete, each of the groups divided from the histories provides values for the quantities of interest, and then the mean and standard deviation of each are calculated from the groups. Finally, a normalized standard deviation is calculated. After several simulations where various numbers of histories were tested, it was decided that the appropriate number of histories for each domain was 1,000,000. Though this number is large and it is known that a higher number of histories leads to a longer run time, this number allowed us to capture the most accurate simulation results and thus was necessary.

2.4 Modeling and Boundary Conditions

Figure 8 shows the schematic of the IR chamber as modeled in Ansys CFX with each part of the geometry labeled. Following this, Figure 9 from SpaceClaim presenting top, bottom, and side views of the configuration consisting of the wafer, the holder it sits on, the tray supporting the wafer and holder, and the paddle that supports them all is shown in detail. The thermocouple can be seen located in the center of the air space inside the paddle. The rest of this section will present in detail what parts of the reactor were omitted for simplification, how each part was modeled, and what boundary conditions were applied. Table 2, Table 3, and Table 4 outline the domain and interface settings in detail where the letter labels are those in Figure 8.



Figure 8 Modeled geometry a) IR chamber walls b) IR lamps c) IR chamber fluid d) reactor process tube e) reactor process tube fluid f) silicon wafer g) paddle h) paddle inner fluid i) thermocouple



Figure 9 Details of wafer, holder, tray, paddle configuration, images used courtesy of ANSYS, Inc.

Table 2 Domain settings

	Domain								
Label	Name	Name Type Material Heat Transfer H		Thermal Radiation	Turbulence Model	First Leg Initialization			
a	IR Chamber Walls	IR hamber Walls Solid Morphology, Stationary Domain Motion, No Mesh Deformation		Thermal Energy	Monte Carlo, Participating Media, 1000000 Histories, Gray Spectral Model, No Scattering Model	N/A	328 K Temperature, Automatic Radiation Intensity		
b			IR C	hamber Flu	uid Boundary				
с	IR Chamber Fluid	IR amber Iuid IR abust Iuid Inid Inid Inid Inid Inid Inid Inid In		Thermal Energy	Monte Carlo, Surface to Surface, 1000000 Histories, Gray Spectral Model, No Scattering Model	SST, Automatic Wall Function	0 U,V,W Velocity, 1 atm Static/Relative Pressure, 328 K Temperature, Medium Turbulence (5% Intensity), Automatic Radiation Intensity		
d	Reactor Process Tube	Solid Domain, Continuous Solid Morphology, Stationary Domain Motion, No Mesh Deformation	Fused Silica	Thermal Energy	Monte Carlo, Surface to Surface, 1000000 Histories, Gray Spectral Model, No Scattering Model	N/A	328 K Temperature, Automatic Radiation Intensity		

Table 2 ((continued)
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e	Reactor Process Tube Fluid	Fluid Domain, Continuous Fluid Morphology, 1 atm Reference Pressure, Non Buoyant, Stationary Domain Motion, No Mesh Deformation	Helium at STP	Thermal Energy	Monte Carlo, Surface to Surface, 1000000 Histories, Gray Spectral Model, No Scattering Model	SST, Automatic Wall Function	0 U,V, Velocity, 0.0062 m/s W Velocity, 1 atm Static/Relative Pressure, 328 K Temperature, Medium Turbulence (5% Intensity), Automatic Radiation Intensity
f	Silicon Wafer (Catalyst)	Solid Domain, Continuous Solid Morphology, Stationary Domain Motion, No Mesh Deformation	Silicon	Thermal Energy	Monte Carlo, Participating Media, 1000000 Histories, Gray Spectral Model, No Scattering Model	N/A	328 K Temperature, Automatic Radiation Intensity
bù	Paddle	Solid Domain, Continuous Solid Morphology, Stationary Domain Motion, No Mesh Deformation	Fused Silica	Thermal Energy	Monte Carlo, Surface to Surface, 1000000 Histories, Gray Spectral Model, No Scattering Model	N/A	328 K Temperature, Automatic Radiation Intensity
h	Paddle Inner Fluid	Fluid Domain, Continuous Fluid Morphology, 1 atm Reference Pressure, Non Buoyant, Stationary Domain Motion, No Mesh Deformation	Air at STP	Thermal Energy	Monte Carlo, Surface to Surface, 1000000 Histories, Gray Spectral Model, No Scattering Model	SST, Automatic Wall Function	0 U,V,W Velocity, 1 atm Static/Relative Pressure, 328 K Temperature, Medium Turbulence (5% Intensity), Automatic Radiation Intensity

Table 2 (continued)

i	TC	Solid Domain, Continuous Solid Morphology, Stationary Domain Motion, No Mesh Deformation	TC	Thermal Energy	Monte Carlo, Participating Media, 1000000 Histories, Gray Spectral Model, No Scattering Model	N/A	328 K Temperature, Automatic Radiation Intensity
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Table 3 Domain boundary settings

	Boundaries								
Label	Domain Name	Location	Туре	Mass and Momentum	Wall Roughness	Heat Transfer	Thermal Radiation	Sources	
a	IR Chamber Walls	Bottom Top Front Side Back Side Inlet Side Outlet Side	Wall	N/A	N/A	Fixed Temperature, 328 K	Opaque, 0.02 Emissivity, 0 Diffuse Fraction	N/A	
b		-	-	11	R Lamps	-			
с	IR Chamber Fluid	IR Lamp Surfaces	Wall	No Slip Wall	Smooth Wall	Temperature, Based on Lamp Power	Opaque, 1 Emissivity, 1 Diffuse Fraction	Radiation Source, Isotropic Radiation Flux, Based on Lamp Power	
		Wall Ends	Wall	No Slip Wall	Smooth Wall	Temperature, 328 K	Opaque, 0.02 Emissivity, 0 Diffuse Fraction	N/A	
d	Reactor Process Tube	Wall Ends	Wall	N/A	N/A	Temperature, 328 K	Opaque, 0.02 Emissivity, 0 Diffuse Fraction	N/A	
е	Reactor Process Tube Fluid	Inlet	Inlet, Subsonic Flow Regime, Medium Turbulence (5% Intensity)	Normal Speed, 0.0062 m/s	N/A	Static Temperature, 328 K	Local Temperature	N/A	
		Outlet	Outlet, Subsonic Flow Regime	Static Pressure, 1 atm	N/A	N/A	Local Temperature	N/A	
f	Silicon Wafer (Catalyst)		N/A						
g	Paddle	Wall End	Wall	N/A	N/A	Fixed Temperature, 328 K	Opaque, 0.02 Emissivity, 0 Diffuse Fraction	N/A	
h	Paddle Inner Fluid	Wall End	Wall	No Slip Wall	Smooth Wall	Fixed Temperature, 328 K	Opaque, 0.02 Emissivity, 0 Diffuse Fraction	N/A	
i	TC	Wall End	Wall	N/A	N/A	Fixed Temperature, 328 K	Opaque, 0.02 Emissivity, 0 Diffuse Fraction	N/A	
Table 4 Interface settings

Interface					
Label	Name	Туре	Heat Transfer	Thermal Radiation	Mesh Connection
a,c	Default Fluid Solid Interface	Fluid Solid	Conservative Interface Flux, No Interface Model	Opaque, 0.02 Emissivity, 0 Diffuse Fraction	GGI (General Grid Interface)
c,d	OutsideTube_insideBox	Fluid Solid	Conservative Interface Flux, No Interface Model	Conservative Interface Flux	Automatic
d,e	insideTubeSolid_insideTubeFluid	Fluid Solid	Conservative Interface Flux, No Interface Model	Conservative Interface Flux	Automatic
e,f	Catalyst_insideTube	Fluid Solid	Conservative Interface Flux, No Interface Model	Opaque, 0.9 Emissivity, 1 Diffuse Fraction	Automatic
e,g	Paddle_insideTube	Fluid Solid	Conservative Interface Flux, No Interface Model	Conservative Interface Flux	Automatic
f,g	Paddle_Catalyst	Solid Solid	Conservative Interface Flux, No Interface Model	Conservative Interface Flux	Automatic
g,h	Paddle_insidePaddle	Fluid Solid	Conservative Interface Flux, No Interface Model	Conservative Interface Flux	Automatic
h,i	TC_insidePaddle	Fluid Solid	Conservative Interface Flux, No Interface Model	Opaque, 0.46 Emissivity, 1 Diffuse Fraction	Automatic

2.4.1 Model Simplifications

When creating a CFD model, making simplifications that cut down on number of elements and therefore computational time is one of the most important steps. Figure 10 shows an image of the reactor inside the NanoProduct lab. The large silver cylinder on the left is the preheater, and the gold box is the IR chamber or RTP furnace. Cooling lines on the sides of the furnace and fans on the top and bottom can be seen in this figure as well. It was decided to neglect the fans, cooling lines, and preheater in the CFD model of the reactor. Instead, the preheater was accounted for using a boundary condition of 328 K as an initial temperature for all domains instead of starting at room temperature. Neglecting the cooling lines and fans potentially has an effect on the heating rates and steady state temperatures for both the wafer and the thermocouple, which is discussed in more detail in the heat loss investigation section. Figure 11 shows the inside of the IR chamber where the process tube is located. Another simplification was neglecting the detail above the arches where the lamps are located, along with changing the lamps from cylindrical to hexagonal which will be discussed in detail in later sections.



Figure 10 Outside of reactor in NanoProduct Lab



Figure 11 Close up of process tube inside of RTP furnace of the reactor

Figure 12 shows the first solid model of the reactor geometry. As discussed previously, the cooling lines, fans, and preheater are neglected. However, the entire process tube was included, along with the helical injector and thermal baffle. In Figure 13, the simplified and final model of the geometry, the parts of the process tube that were outside of the IR chamber were neglected. This was partly to cut down on the size of the model, but also because the radiative heating inside of the IR chamber was the main focus of this project. It is also important to note that the helical

injector adds a lot of complexity to the model. This is because a very small fluid area must be added inside it, and this fluid must then flow through several holes around the last coil and also out of the end. In the future, the rest of the process tube and its components and the preheater that surrounds it could be included.



Figure 12 Original full model of reactor geometry, image used courtesy of ANSYS, Inc.



Figure 13 Simplified (final) model of reactor geometry, image used courtesy of ANSYS, Inc.

2.4.2 IR Chamber Walls

The walls of the IR chamber of the CVD reactor are gold coated. In the model, gold is used as the bulk material for this geometry. The outer surfaces of the walls are modeled as having fixed temperature of 328 K and are opaque with an emissivity of 0.02 and diffuse fraction of zero. The values for emissivity and diffuse fraction are chosen as these values represent a mirror, and the walls in the actual reactor are gold coated to reflect the radiative heat from the IR lamps. The inner surfaces of the IR chamber that are in contact with the fluid inside the chamber are modeled using a fluid-solid interface in Ansys CFX. In this type of interface, there are settings for mass and momentum, wall roughness, and heat transfer. In this case, mass and momentum was set to no slip wall, thus using the no slip boundary condition. The wall roughness is set to smooth wall, as the inner chamber walls are smooth in reality. Lastly, the heat transfer is set to conservative interface flux, which is the only available option for this interface.

2.4.3 IR Chamber Fluid

In the physical CVD reactor, the fluid inside of the IR chamber surrounding the lamps and the process tube is air. Therefore, in the model this domain's material is set to air at STP. Since this is a fluid domain, a turbulence model must be selected. In this case, the Shear Stress Transport (SST) was determined to be best. For the purpose of these simulations, the inlet and outlet of this domain are set to walls with the same settings as the IR chamber walls.

The IR lamp boundary conditions are also set in this domain, since they are modelled as voids and not actually present in the geometry, which will be discussed in more detail in the following section.

2.4.4 IR Lamps

Several different lamp geometries were created and tested, but the most studied geometries were cylindrical and hexagonal shaped lamps. The shape of the lamps was changed from cylindrical to hexagonal to reduce the mesh around the lamps. It was noticed that the cylindrical shape caused a much finer mesh than necessary due to capturing the curves of the cylindrical shape, so hexagonal lamps were created. When creating the hexagonal lamps from the cylindrical lamps, it was important to keep the surface area the same so that the results from both the cylindrical and hexagonal lamps could be compared to make sure that the results were the same. It was known that the surface area of the five millimeter diameter cylindrical lamps, which the hexagonal lamps were based off of, had a surface area of 2960.95 mm², so the dimensions of the hexagonal lamps were determined based off of this. The hexagonal lamps have a side length of 2.6212 mm, which yields a 2960.9263 mm² surface area, which is very close to the cylindrical lamp surface area.

The hexagonal lamps eliminated the need for the curves to be captured and allowed the mesh to be refined using face meshing on each of the six sides of the hexagon. A mesh convergence study was performed to determine the best face meshing element size. The starting point was an element size of 2.6212 mm, which is the length of one of the six sides of the hexagon. The first refinement divided this face meshing by 1.5, giving an element size of 1.7474 mm. The second refinement divided the face meshing by two, with an element size of 1.3106 mm. The third refinement divided the face meshing by 1.4 creating an element size of 1.8723, and lastly the fourth refinement divided the face meshing by 2.25 creating an element size of 1.165 mm. It was determined that the third refinement with an element size of 1.8723 mm on each face of the hexagonal lamps produced the best results while still significantly lowering the number of elements from the cylindrical lamp model. This lamp meshing was then adopted for all following simulations where the hexagonal lamps were used. Figure 14 shows a comparison of the mesh around the original cylindrical lamps and the hexagonal lamp mesh refinements. These meshes, and all others mentioned in this work, were generated using the Fluid Flow (CFX) Analysis System in Ansys Workbench version 2021 R2.



Figure 14 a) original cylindrical lamp mesh, 574,978 elements b) original hexagonal lamp mesh, face meshing element size 2.6212 mm, 275,719 elements c) hexagonal lamp mesh refinement one, face meshing element size 1.7474 mm, 400,441 elements d) hexagonal lamp mesh refinement two, face meshing element size 1.3106 mm, 497,519 elements e) hexagonal lamp mesh refinement three, face meshing element size 1.8723 mm, 327,827 elements f) hexagonal lamp mesh refinement four, face meshing element size 1.165 mm, 555,186 elements. Images used courtesy of ANSYS, Inc.

It is also important to note that all lamps are modeled as "voids" to reduce the total element count of the model. The lamps are physically present in the original geometry, and then removed before the model is imported into CFX. This creates lamp-shaped holes in the fluid area inside of the IR chamber. The lamp boundary conditions are then applied to the faces of the fluid that would be touching the lamps if they were present. A fixed temperature and radiation source of isotropic radiation flux are applied to these faces to simulate a specific lamp power. The values for lamp temperature and flux are described in detail in the results section.

2.4.5 Reactor Process Tube

In the reactor, the process tube is made of fused silica, thus this is the material that this domain is set to in the simulations. Determining the absorption coefficient of this material was the biggest challenge and many values were tested, but it was decided that a value of 0.1 1/m yielded results that most closely matched experimental values. The ends of the process tube are set to the same boundary conditions as the IR chamber walls. A fluid-solid interface is defined at the outer wall of the process tube that is in contact with the IR chamber fluid. Here, both the heat transfer and thermal radiation options are set to conservative interface flux. While there are other options available for this interface, conservative interface flux was determined to be the best option, as it implies that the heat transfer or thermal radiation will flow between that boundary and the boundary on the other side of the surface²¹. Therefore, this allows heat and radiation to flow from the fluid surrounding the tube to the process tube.

2.4.6 Reactor Process Tube Fluid

The fluid inside the process tube is set to helium at STP, matching the helium that is injected into the process tube in the actual CVD reactor. Again, SST is used as the turbulence model. Here, there is an inlet and an outlet. The inlet is set to a normal speed of 0.0062 m/s with a static temperature of 328 K. The outlet has a static pressure of one atm. The fluid-solid interface between the process tube and the process tube fluid is again set to conservative interface flux.

2.4.7 Silicon Wafer/Catalyst

In reality, there is a catalyst present on top of the paddle that is made of silicon, so the material for this domain is set to that. The mesh of the wafer is also very fine, since this is one of the most important parts of the geometry and one of the goals of this model is to capture the temperature distribution on the wafer as accurately as possible. There is a fluid-solid interface present between the catalyst and the fluid inside of the process tube, where the heat transfer is set to conservative interface flux. The thermal radiation, however, is set to opaque with an emissivity of 0.9 and diffuse fraction of one, and these values were determined through several simulations, This is not quite a blackbody which would have an emissivity of one, but very close which accurately represents the silicon wafer.

2.4.8 Paddle

The paddle in the reactor is made of fused silica, and therefore is modeled as such. As in the other solids, the end of the paddle that is not inside the reactor has the same settings as the IR chamber walls. The catalyst rests on the paddle, so there must be a solid-solid interface defined there, and conservative interface flux is used for both heat transfer and thermal radiation.

2.4.9 Paddle Inner Fluid

The fluid inside the paddle is set to air at STP, as the inside paddle fluid in the reactor is also air. This fluid does not have an inlet, and the end of the fluid that is not inside the reactor is again set the same way as the IR chamber walls. Since this is a fluid domain, the turbulence model is again set to SST. The interface between the solid paddle and fluid inside the paddle is again set to conservative interface flux for both the heat transfer and thermal radiation options.

2.4.10 Thermocouple

The thermocouple arrangement inside of the reactor consists of three K-type thermocouples that start at the entrance of the process tube. The ends of these thermocouples are staggered by approximately one inch, and the longest ends near the middle of the silicon wafer. Each of these thermocouples consist of a Pyrosil D sheath, MgO insulation, one thermoelement made of alumel, and one thermoelement made of chromel. Since the model was already very complicated before the thermocouple was introduced, it was decided to model the thermocouple as one bulk material instead of modeling each of the elements. It was also decided to model just one thermocouple instead of all three. The thermocouple is surrounded by an air space inside of the paddle, and the end of the thermocouple is just under the middle of the silicon wafer. A schematic of this is shown in Figure 15.



Figure 15 Thermocouple schematic

2.4.10.1 Material Properties Investigations

The most challenging aspect of modeling the thermocouple was determining its material properties. It was known that the thermocouple was type K, made up of a Pyrosil D sheath, MgO insulation, one wire made of alumel, and one wire made of chromel. The material properties for all of the components except for the Pyrosil D sheath, were well documented. As stated previously, it was decided to model the thermocouple as one solid material instead of modeling all of the individual components, as that would add too much complication to the model that was already very detailed. To do this, an area weighted average calculation of the materials was performed, using a diagram of a type K thermocouple. The percentage of the total thermocouple area for each component was calculated, and then for each material property (density, specific heat, thermal conductivity, and molar mass) the material property's value was multiplied by the percentage and then added together to get the final material property. This method was also used by Nakos²² for determining thermocouple material properties in the same way.

Once the first set of thermocouple material properties were obtained, several simulations were completed at the same lamp power value to test each material property. One property was changed at a time and then compared to experimental results to determine which value was the most accurate. Emissivity values of 0.46, 0.66, and 0.86 were tested, and this range was obtained from Nakos²² and Brundage et al²³. The temperature vs time and temperature vs length plots were evaluated, and it was determined that 0.46 was the best emissivity value, as shown in Figure 16.



Figure 16 Thermocouple emissivity investigation

The next material property that was investigated was density. Values of 5880 kg/m³ and 6576 kg/m³ were tested, and it was determined that 6576 kg/m³ was the most accurate value as shown in Figure 17. The value of 5880 kg/m³ was obtained from Brundage et al²³ and 6576 kg/m³ was calculated using the area weighted average method mentioned above.



Figure 17 Thermocouple density investigation

The specific heat of the thermocouple was also investigated. The calculated value was 618 J/kgK, and 696 J/kgK from Brundage et al²³ was also tested. As shown in Figure 18, it was determined that the 618 J/kgK value was the most accurate.



Figure 18 Thermocouple specific heat investigation

The thermocouple material property that was investigated most extensively was the thermal conductivity. The original calculated value was 67 W/mK, and values of 1.7 W/mK and 30 W/mK were also tested. The thermal conductivity of 1.7 W/mK was obtained from Brundage et al²³ and 30 W/mK was a chosen value between 1.7 and 67 for the purpose of testing. Neither of these values were satisfactory, so the thermal conductivity was recalculated using new values but the same area weighted average method. The new values for each component were obtained from Yilmaz²⁴. It was decided that these values closely represented the model thermocouple because their sheath is made of Inconel 600, while the thermocouple in the reactor has a sheath made of Pyrosil D, and their material properties are very similar as they both consist of about 70% nickel and about 20% chromium. The insulation material used in Yilmaz²⁴ is MgO which is the same as the reactor thermocouples', and their thermoelements are alumel while the reactor thermocouples' are alumel

and chromel. So, using the thermal conductivity values for each element from Yilmaz²⁴, a new area weighted average was created, yielding a new thermal conductivity of 8.67 W/mK. From Figure 19, it is evident that this thermal conductivity value produces the best results. Though the temperature vs time plot would indicate that each of these values are relatively the same, plotting temperature along the length for a given point in time shows that 8.67 W/mK yields the most uniform temperature results. The importance of this spatial uniformity in thermocouple temperature measurement is explored further in the results section.



Figure 19 Thermocouple thermal conductivity investigation

2.5 Mesh Convergence

To ensure that the silicon wafer temperature results were independent of the mesh size, a mesh convergence study was conducted. The main focus was the area of the fluid inside the process tube that came in contact with the silicon wafer. Face meshing was performed on the six faces of this fluid area that came in direct contact with the six faces of the wafer. The first refinements

changed the face meshing element size from 0.5 mm to 0.3 mm, the second changed the size to 0.175 mm, and the third and final refinement changed the face meshing element size to 0.1 mm. Each of these refinements more than doubled the number of elements in the fluid inside the process tube. Nothing else was changed in the simulations to ensure that the differences in wafer temperature were due to these refinements and nothing else, and all simulations were conducted at the same lamp power. It was determined that the second refinement was sufficient since there was almost no change in the wafer temperature from refinement two to refinement three, as shown in Figure 20, Figure 21, Figure 22, and Figure 23. It is also important to note that a mesh convergence study was not necessary for the thermocouple, as the temperature values were independent of mesh size and time stepping, as the values did not change if the time step or mesh size was changed.



Figure 20 Mesh refinements, images used courtesy of ANSYS, Inc.



Figure 21 Mesh convergence temperature vs time



Figure 22 Wafer temperature at 6 seconds



Figure 23 Wafer temperature at 14 seconds

3.0 Results and Discussion

3.1 Validation of Lamp Boundary Condition Modeling

The most important task in modeling the IR chamber was determining how to model the thermal boundary conditions applied to the IR lamps. The main objective was to determine a relationship between the lamp temperature and flux with respect to specific lamp powers. A similar relationship is presented by Coaton²⁵, who provides a relationship between lamp envelope temperature and power in watts. In Coaton²⁵, envelope refers to a short tube made of fused quartz that is sealed at both ends and contains a tungsten filament and halogen gas. This is very similar to the fused silica IR lamps used in the reactor, so this paper was used as a starting point to determine the model's lamp boundary conditions. In this method (original), zero watts (W) represents 0% lamp power and 1600 W represents 100% lamp power. The assumption is made that 1600 W is the maximum power for the reactor's IR lamps based on data from the lamp manufacturer. Coaton²⁵ also presents data for 389 W, 715 W, 1124 W, and 1412 W, and this is used to determine which wattage corresponds to which power percentage by dividing the respective wattage by 1600 W and multiplying by 100. Coaton²⁵ provides data for envelope temperature at these wattages, and a relationship between lamp power and envelope temperature is determined from plotting temperature vs wattage and creating a linear trend and equation from the data. This equation can then be used to obtain a lamp temperature for any chosen power value. The net radiative flux per lamp is then calculated using Stefan-Boltzmann law to calculate the thermal energy radiated from the lamp, and then this value is subtracted from the given power in watts. The flux values are then plotted against their respective power, a linear trend is created, and

then the resulting equation is used to calculate lamp flux values for any other power percentage as was done with lamp temperature.

The next method (method one) is adjusted from the original where zero watts is now 0% power and 1412 W is 100% power. Another adjustment is that 0% power now has a lamp temperature of 526 K and a flux of zero, where in the previous method 0% power had a lamp temperature of 298 K. This assumption is justified based on the fact that there is a preheater present before the IR chamber, thus 0% lamp power does not necessarily mean that the IR chamber starts at room temperature. Power percentages are calculated in the same way as the previous method with the adjusted range, and are plotted against the envelope temperatures given by Coaton²⁵ for each respective wattage. This again creates a trend and a linear equation that can be used to calculate lamp temperature at any power percentage. The lamp flux is calculated the same way as the previous method but again adjusted for this new range.

Method two considers 389 W to be 0% power and 1412 W to be 100% power. Method three uses 389 W as 0% power and 1600 W as 100% power. Both the lamp temperature and lamp flux were calculated using the same process as the previous method and were adjusted for their respective ranges.

Multiple simulations at different lamp power values were conducted for each of these methods, and it was determined that method one provided the best agreement with experimental results. A plot of the experimental and simulation temperature at 126 seconds is shown in Figure 24. Here, it can be seen that the method one (simulation) values match well with the experimental values, and their trend lines are similar as well.

In later simulations, better agreement between simulation and experimental temperatures was achieved through several minor changes to the chosen method. First, the initial fixed

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temperature of each domain was changed from 298 K to 328 K to better represent the preheater present in the reactor before the IR chamber. Second, the lamp flux value for each power was multiplied by a radiative efficiency term. This term was obtained from Jenkins et al¹³, which provides a relation between radiative efficiency and lamp filament temperature. These values were adjusted for the purpose of this project and range from 0.5 (50%) for 0% power and 0.9 (90%) for 100% power.



Figure 24 Temperature at 126 seconds

3.2 Thermocouple Spatial Uniformity

When the results from a simulation are analyzed, the top face of the wafer is chosen and an area average of temperature over this face is calculated. This area average is then plotted vs time. For the thermocouple, the same method is used at the end of the thermocouple that is present inside paddle just under the center of the wafer, as shown in the thermocouple schematic in Figure 15. However, spatial uniformity in the thermocouple temperature results can also be demonstrated by plotting the thermocouple temperature along its length for several points in time. The chart in Figure 25 provides an example of this for 15% lamp power at the last time step of each of the simulation legs. The contour plots of the thermocouple, also shown in Figure 25, for 15% lamp power at the last time step of each of the simulation legs further exemplify this spatial uniformity.



Figure 25 Thermocouple temperature vs length at end of leg for 15% power, images used courtesy of ANSYS,

3.3 Stitching Time Stepping Scheme to Compare Wafer Temperature to Thermocouple Temperature

Deciding on an appropriate time step that accurately captures simulation data while also taking the least amount of computation time is important in any CFD project. A "stitching" method was used to complete simulations for longer durations. This was so that the results of a simulation could be checked intermittently, and if any issues were present it could be adjusted early on before waiting days for completion. The first few seconds of the simulations experience the most dramatic rise in temperature, thus it was hypothesized that zero seconds to two seconds should have a very small time step of 0.0025 seconds. To "stitch" this first simulation to the next one, the last time step of this leg is used as the initial values for the next leg. The same stitching method is used for all following legs where the last value of the previous leg is used as the initial value for the next leg. The time stepping scheme used for the next leg multiplied the time duration of the previous leg by two and the time step by two or four. So, the second leg was two seconds to six seconds with a time step of 0.01 seconds, the third leg six seconds to 14 seconds with a time step of 0.04 seconds, the fourth leg was then 14 seconds to 30 seconds with a time step of 0.08 seconds. The final leg was 30 seconds to 62 seconds with a time step of 0.16 seconds, and this time step was determined to be the largest that can be used without compromising results for the wafer temperature. Thus, for all simulations that were run longer than 62 seconds a time step of 0.16 seconds was used, if the wafer temperature was the main focus. These time stepping scheme values were determined from conducting many simulations and decided the largest time step for each leg that could be used without effecting the wafer temperature.

This study also demonstrated that thermocouple temperature was independent of time step but wafer temperature was not. Figure 26 compares different time stepping schemes where it can be shown that the thermocouple temperature does not change with time step size, but the wafer temperature does. Therefore, simulations where only the thermocouple temperature were considered could use time steps larger than 0.16 seconds. This also means that these simulations could be run for a longer period of time since they took less computational time. In general, when analyzing thermocouple temperature only and not wafer temperature, the time duration and time step were doubled for each leg. For example, zero seconds to 126 seconds had a time step of 0.16 seconds, 126 seconds to 378 seconds had a time step of 0.32, and so on to the desired simulation time. This scheme was used for 10% and 5% power up to a 0.64 second time step, as any larger than that caused issues with Ansys CFX. For 15% lamp power, 0.16 second was used for the first two legs.



Figure 26 Time step investigation

3.4 Model Validation: Comparison with Experimental Results

The main method of validating the simulation results was to compare them with experimental results at the same power percentages. Since the reactor outputs temperature data read from the thermocouples present inside the IR chamber, it was decided that reading the simulation temperature from the end of the thermocouple would most accurately represent experimental results. Figure 27 and Figure 28 show the simulation thermocouple temperature compared to the experimental thermocouple temperature at lamp power values of 5%, 10%, and 15%. Contour plots generated in Ansys CFD-Post are also provided for several points in time for 5% and 15% power. A zoomed in temperature contour plot of the thermocouple and its surrounding air space is also shown.



Figure 27 Experimental thermocouple temperatures



Figure 28 Simulation thermocouple temperatures i) plot of thermocouple temperature vs time for 5%, 10%, and 15% lamp power ii) contour plots of IR chamber for 15% lamp power at specified points in time iii) contour plots of IR chamber for 5% lamp power at specified points in time iv) zoomed in image of thermocouple contour plot for 5% lamp power at 800 seconds. Images used courtesy of ANSYS, Inc.

The wafer temperatures from the same simulations are presented in Figure 29. Though time step independence for the wafer has not yet been achieved, these simulations are still valuable. They allow us to examine the temperature distribution on the top side of the wafers, as shown in the contour plots in Figure 29. It can be seen that the legend has a very small range, as temperature uniformity is extremely important in growing CNTs. The contour plots shown in c, d, and e in Figure 29 show the dependence of the wafer temperature profiles on lamp power, as the wafer temperatures are much lower for 5% power than 10% or 15% lamp power. It is also important to note that the wafer is very small, at 10 millimeters in height and length 0.525 millimeters thick.

The plot in Figure 30 gives more insight into the temperature nonuniformities on the surface of the wafer shown in the contour plots of a, b, and c in Figure 29. Here, temperatures at the edge of the wafer and at the middle of the wafer at 5%, 10%, and 15% lamp power for several points in time were obtained. The temperature difference across the wafer is calculated using an average of the four corner temperatures, and an average of five points in the middle of the wafer. These averages are then subtracted, creating a temperature difference, or Delta T as labeled on the plot, across the wafer. This shows that not only is there temperature nonuniformity at earlier times in the simulation (50 and 110 seconds), but also at steady state (800 seconds). This is likely due to the fact that a cold-wall reactor is used, so the edges of the wafers have lower temperatures due to the cooling that is occurring on the outer walls of the reactor. It can also be observed that the temperature difference increases as power percentage increases. The implications of these temperature nonuniformities on the wafer surface include catalyst nonuniformity and nonuniformity in CNT growth. In the future work section, this temperature distribution is explored in more detail.



Figure 29 Simulation wafer temperatures, images used courtesy of ANSYS, Inc.



Figure 30 Change in temperature across the surface of the wafer for 15% lamp power at several points in time

It is also important to note what the results presented here show that previous works do not. Logerais et al² presents a similar RTP CVD model and shows a relation between lamp power and wafer temperature, but does not provide plots of the temperature distribution on the wafer. As discussed previously, these spatiotemporal plots of temperature on the wafer can provide important information about nonuniformities during CNT growth. This paper also mentions the use of a thermocouple for temperature measurement, but does not include it in the model.

3.5 Heat Loss Investigation

To account for some of the differences between the experimental and simulation temperatures, an investigation of the heat losses in the IR chamber was conducted. This was done in post-processing, as Ansys CFX offers many thermal values that can be plotted for any domain from the simulation in Ansys® CFD-Post, Release 2021 R2. In this case, the values considered were wall heat flux, wall conductive heat flux, wall convective heat flux, wall absorbed radiation flux, and wall radiative heat flux. Wall heat flux refers to the total heat flux into the specified domain, which includes the wall conductive and wall convective heat flux values²⁰. Wall conductive heat flux and wall convective heat flux refer to the heat flux from conduction and convection heat transfer respectively. Wall absorbed radiation flux represents the absorbed heat flux due to radiation. Wall radiative heat flux represents the net radiative energy flux leaving a specified boundary. It is computed as the difference between the radiative emission and the incoming (absorbed) radiative flux. Though not included in Ansys, the wall emitted radiation flux was also considered and obtained by subtracting the wall absorbed radiation flux values from the wall radiative heat flux values. An area integration method was used, thus outputting values in watts (W) instead of W/m^2 , and therefore the values will be referred to as heat instead of heat flux going forward. Each of these values were plotted over time for the fluid and solid side of the thermocouple, the fluid and solid side of the inner walls of the IR chamber, and the outer walls of the IR chamber which only have a solid side. It was decided to conduct this investigation for 5% lamp power, but any of the three lamp powers discussed in the results could be used for the same purpose. It is also important to note that this investigation was conducted only for the first leg of the simulation from zero seconds to 126 seconds. This is because the most drastic heating occurs during this time frame.

Figure 31 shows the heat loss investigation results for the IR chamber outer walls. These plots show that the only mode of heat transfer on the outer walls is conduction, and that the heat losses eventually reach a steady state. There is no convection present on the outer walls because the model did not include the cooling lines or fans present in the actual reactor in order to simplify the CFD model. Not including the convective cooling on the outer walls in the model could possibly be delaying the steady state and may be why the model overestimates the final thermocouple and wafer temperatures and underestimates the heating rates for the thermocouple and wafer. Despite what the plot appears to present, the wall radiative heat is zero. This is known because the boundary conditions set on the outer walls of the reactor represent a mirror with an emissivity of 0.02 and a diffuse fraction of zero. Examining the plot on the left, it can be concluded that the reason for the noise giving the wall radiative heat a value other than zero is the noise from calculating wall absorbed and wall emitted heat. There is also the factor of numerical error which is a factor in any CFD model, especially one performing complex radiation calculations.



Figure 31 IR chamber outer walls heat loss investigation

Figure 32 shows the heat loss investigation results for the solid side of the fluid solid interface present on the inner walls of the IR chamber. Here, it can be seen that a steady state is reached very quickly, unlike the outer walls. This is because the assumptions made for the outer walls do not affect the inner walls. There is convection heat transfer present on the inner walls, however convective heat is not shown on the plot since only the solid side of the boundary is being considered. The existence of convection on the inner walls, though it is not shown for the solid side, is likely the reason that the inner walls reach a steady state faster than the outer walls. The inner walls also have the mirror boundary condition, meaning that the radiative heat should be zero. The large spikes and noise that cause the appearance of radiative heat in the plots are the same as those described when discussing the IR chamber outer walls.



Figure 32 IR chamber inner walls solid side heat loss investigation

Figure 33 shows the heat loss investigation results for the fluid side of the IR chamber inner walls. This plot shows that there is convection heat transfer on the inner walls. As described above, the existence of this convective heat is likely the reason for a steady state being reached faster than the outer walls. Here, there is no noise from the radiative heat transfer, and the value is not zero.

It can be seen from the plot that the radiative and convective heat added together amounts to the total wall heat.



Figure 33 IR chamber inner walls fluid side heat loss investigation

Lastly, Figure 34 shows the heat loss investigation results for the fluid side (left) and solid side (right) of the thermocouple fluid solid interface. On the fluid side, the net heat transfer is negative, due to convection cooling being larger than the radiative heat value. On the solid side, the radiative heat is zero, thus the only mode of heat transfer is conduction. Thus, the solid side dissipates heat through conduction. The line for wall conductive heat matches exactly with the line for wall heat which is the reason it is not seen on the plot.



Figure 34 Thermocouple fluid side (left) and solid side (right) heat loss investigation

3.6 Future Work

Now that a working model of the IR chamber has been created, this model can be used for many other simulation projects. The first task will be to obtain wafer temperature data that is independent of time step. New wafer holder designs can also be investigated, several of which have already been created in SpaceClaim. The wafer material can also be changed from silicon, and the fluid that is injected into the process tube can be changed from helium to argon to investigate these effects on catalyst formation. As mentioned previously, temperature uniformity on the surface of the wafer is very important. This can be investigated more in later simulations by changing the boundary conditions at the edges of the wafer, changing the tray and wafer holder design, or changing the material properties of the wafer. The effect that the CNTs have on the wafer temperature can be investigated by adding CNTs to the model on top of the wafer. Since these are black and absorb a lot of radiation, it is expected to effect the temperature of the catalyst under them. Also, new geometry can be created that includes the preheater. This preheater can be
modeled and added outside of the IR chamber, though many of the preheater's effects are already accounted for in the current model through the fixed temperature boundary conditions. As mentioned previously, the cooling lines and fans present on the outside of the IR chamber can be added to the model to further investigate the effects of convection cooling on the wafer temperature uniformity. Components of the process tube that were neglected, such as the thermal baffle and helical injector, can also be added to investigate their effects.

4.0 Conclusions

In this thesis, a CFD model that captures the rapid thermal processing within the IR chamber of the NanoProduct Lab's custom CVD reactor used for catalytic growth of carbon nanotubes was presented. The CVD process was introduced, as well as several types of CVD reactors and a description of the use of RTP in CVD. The importance of modeling CVD reactors to grow CNTs was presented. A description of the actual CVD reactor and equipment was provided as well as a description of experiments and previous works with similar reactors were reviewed. Previous IR chamber models were investigated, however this work proved to be unique and new. The material properties used were discussed, as were the governing equations used in Ansys CFX. It was determined that the best radiation model in Ansys CFX for this case was Monte Carlo with a transfer mode of surface to surface or participating media depending on the domain. Simplifications from the actual reactor and earlier full model of the geometry were explored. The boundary conditions present in each domain were outlined and the reasoning behind any assumptions that were made was provided. Modelling the thermocouple accurately presented many challenges, such as determining the correct material properties. A mesh convergence study was conducted to determine the level of mesh refinement needed to save the most computation time but not compromise the results. Modeling the IR lamps required many tests to determine the best geometry, mesh density, and boundary conditions. Several methods were tested to model the lamp boundary conditions, and the best method was selected. Time step and mesh independent results for the thermocouple temperature were demonstrated and spatial uniformity for these temperature results was also shown. The model shows good agreement with experimental temperature results obtained for the power percentages of 5%, 10%, and 15%. An investigation of the heat losses was also performed, leading to more insight on the temperature nonuniformities present on the wafer. It was determined from this investigation that not taking into account the cooling on the outside walls of the IR chamber are one of the main contributing factors in the difference between experimental and simulation temperatures. In future work, this is something that can be further explored, as well as other modifications to this model. Overall, the model has proved to be useful in exploring temperature nonuniformities leading to nonuniform CNT growth.

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