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Doctoral Education in Chemistry: Faculty perspectives on programmatic elements' goals and outcomes

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This qualitative study investigates the goals and outcomes of the individual programmatic elements within US chemistry doctoral programs, based on faculty perspectives. Forty-six faculty participants were interviewed using an interview protocol that was refined through iterative input and consensus building. Faculty perspectives in this study identifies several programmatic elements—such as research, coursework, lab rotations, candidacy process, and teaching assistantship—and explores the goals and outcomes of each. While the program's structure aims to incorporate essential workforce skills as explicit goals and outcomes, findings indicate that this integration often remains questionable. Further analysis of the goals and outcomes yielded three main insights: there is a misalignment between stated goals and enacted practices, necessitating a holistic reform approach to align goals of programmatic elements with students' career goals and program goals; the structure of some programmatic elements often causes stress and frustration, highlighting the importance of improved integration and support; significant issues with certainty of the goals and outcomes of programmatic elements were identified, suggesting systemic problems that could lead to ineffective education. Addressing these issues through enhanced clarity, alignment, and practical training is vital for improving the experience of doctoral education in chemistry and better preparing students for their careers. While this study focused on US chemistry doctoral programs, the findings offer a framework for improving doctoral programs by addressing misalignments, unclear goals and outcomes, and the integration of real-world skills, providing insights that are applicable across diverse global educational contexts.

Introduction

Science, technology, engineering and math (STEM) education especially, doctoral education in chemistry (DEC) is essential due to its immense contribution to society (Educational Testing Services and Council of Graduate Schools, 2010; Carnevale *et al.*, 2011; Press and Maxine Savitz, 2012; Andrea Widener, 2016). DEC has played a crucial role in the training of various scientists and professionals and contributed to the production of numerous technological innovations (Golde and Walker, 2006; Kuck *et al.*, 2007; Nolan *et al.*, 2008; Press and Maxine Savitz, 2012; Wilson *et al.*, 2014; Andrea Widener, 2016; Stockard *et al.*, 2022). However, research shows that career success for chemists depends not only on obtaining a degree, but also on demonstrating strong work values, independence, and specific work interests (Carnevale *et al.*, 2011). Our previous findings emphasize that one of the primary goals of DEC is to equip students for their careers (Donkor *et al.*, 2024) and a prior study identified specific knowledge and skills that Ph.D. chemists need in their professional careers (Cui and Harshman, 2020).

Misalignment of doctoral education and workforce skills

Despite the primary focus on preparing students for their careers within doctoral education, many national reports and studies highlight a misalignment between the workforce skills developed by doctoral students during their graduate studies and those required for their careers (Educational Testing Services and Council of Graduate Schools, 2010; Presidential Task Force on Innovation in the Chemical Enterprise, 2011; Council of Graduate Schools and Educational Testing Services, 2012; Press and Maxine Savitz, 2012; National Academies of Sciences, 2018; Busby and Harshman, 2021; Cui and Harshman, 2023). This misalignment suggests that while doctoral programs focus on deep academic knowledge, they may overlook practical skills needed in the workforce. Consequently, research has shown that employers encounter challenges recruiting graduates due to deficiencies in essential workforce skills (Noah and Aziz, 2020). Further research highlights that even though most doctoral degree holders will not stay in academia, they are unsure what skills they need for careers outside academia and how to

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Supplementary Information available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x

acquire them (Kehm, 2020; Donkor *et al.*, 2024). This reinforces the question of whether doctoral programs effectively prepare students for their intended goals, as debates highlight differing views on success measures—employment rates versus the need for reform due to issues like inadequate career preparation, over-specialization, and graduate oversupply, with studies calling for comprehensive reform in Ph.D. programs (Kwiram, 2004; Ostriker *et al.*, 2011; Presidential Task Force on Innovation in the Chemical Enterprise, 2011; Taylor, 2011; Committee on Challenges in Chemistry Graduate Education *et al.*, 2012; Rovner, 2012; Rovner and Wang, 2015; Ashby and Maher, 2018; Cui and Harshman, 2020, 2; Busby and Harshman, 2021; Harshman, 2021).

The foundations of chemistry doctoral programs

The US chemistry doctoral program's structure has remained consistent for decades, with key elements like research, coursework, and research advisors (among others) playing significant roles (Mohrig, 1997; Committee on Professional Training, 2008; Harshman, 2021; Donkor and Harshman, 2023). This consistency suggests that these elements either effectively meet their intended goals or persist due to resistance to change, despite potentially not serving their intended purposes (Chandler, 2010; Aldiabat *et al.*, 2022). For instance, prior research highlights significant misalignments in the perspective of policy agents (faculty members) and actual policies (graduate handbook) within doctoral education. Nardo (2024) effectively demonstrated misaligning and/or conflicting statements between faculty members and the policies they claimed to uphold revolving around key milestones like admissions, coursework, candidacy processes, and dissertation defense. This causes ambiguous expectations and creates boundaries for students' success, ultimately prioritizing legitimacy (granted access from those already in power) over learning (Nardo, 2024). Despite the importance of the programmatic elements there is a lack of research on how these elements contribute to the program's overarching goals (Donkor and Harshman, 2023). Previous studies highlight the need for reform in the elements as there may be a need for complete, moderate, or minor adjustments (Busby and Harshman, 2021; Harshman, 2021). Therefore, investigating the goals and outcomes of these elements is essential to better align them with the program's overarching goal(s).

Purpose of study

This qualitative study focuses on gaining insights regarding the goals and outcomes of the individual programmatic elements within the DEC program. For the purpose of this study goals are defined as what students are expected to know, understand, and accomplish (intended outcomes), while outcomes are specific actions or behaviours that demonstrate the achievement of these goals (what students actually gain) (Wiggins *et al.*, 2005; Donkor and Harshman, 2023). We seek to understand how these elements contribute to the overarching program goal(s) of DEC. This purpose led to the following research questions:

i. From faculty perspective, what are the goals (intended outcomes) and outcomes (actual outcomes) of the individual programmatic elements of doctoral education in chemistry?
ii. What insights can be drawn from the goals and outcomes of the individual programmatic elements?
iii. How well do these goals and outcomes align with the reported overall goal (preparing students for careers)?

This study is a part of a larger research project that aims to examine the unique perspectives of faculty members towards DEC from a comprehensive standpoint (Donkor *et al.*, 2024). While the overall project delves into faculty perspectives on various aspects of DEC, the current study specifically focuses on the aforementioned research questions.

Theoretical framework: Teacher-Centred Systemic Reform

Our focus on faculty in DEC is guided by the teacher-centred systemic reform (TCSR) framework. TCSR acknowledges the interaction between teacher (faculty advisor in this context) thinking, personal factors, and contextual factors that influence important enacted practices for educational reform (Woodbury and Gess-Newsome, 2002; Gess-Newsome *et al.*, 2003; Popova *et al.*, 2021; Reinholz *et al.*, 2021; Southard *et al.*, 2021). Faculty perspectives (teacher thinking) on the goals and outcome of the programmatic elements is essential, as they play a key role in the training and mentoring of doctoral students (Council of Graduate Schools in the US Washington, DC, 1991; Mauch and Park, 2014; Ashby and Maher, 2018; Harshman, 2021). Personal factors include demographics, mentoring/teaching experiences, faculty member's level of preparation among others, while contextual factors encompass institutional and cultural dynamics (Woodbury and Gess-Newsome, 2002; Popova *et al.*, 2021). Enacted practices encompass applied mentoring and/or teaching methodologies, approaches, and actions undertaken by faculty with an explicit aim of moulding the educational experiences of students.

Understanding the interdependency of teacher thinking, personal and contextual factors, and enacted practices is vital for effective reform. Although not originally intended for DEC, previous studies, emphasize the model's significance in offering guidance for reform initiatives (Woodbury and Gess-Newsome, 2002; Popova *et al.*, 2021).

Methods

Positionality statement

As research scientists, we recognize that our diverse backgrounds, identities, perspectives, beliefs, and previous experiences greatly impact every aspect of our scientific work (Wilson *et al.*, 2022). Therefore, we believe it is important to reveal key aspects of our identities and perspectives that are closely related to the work being conducted, and to be transparent about methods which were used to mitigate the impact of those perspectives. The study's initial design was conducted by author JH who is a research faculty with a specialty in DEC (Harshman, 2021). This expertise equips him with a comprehensive understanding of the current state of DEC. JH holds the belief that the current challenges facing DEC call for reform. Nevertheless, he diligently abides by the present practices of modern DEC on a daily basis. Author BD, a graduate student, finds her current academic path closely intertwined with the goals and outcomes of the programmatic elements. These programmatic elements significantly contribute to DEC's overarching goal, the subject currently under investigation. This connection increased her interest in the study and moulded her perspectives regarding the intended purpose. Author MAC (a postdoctoral fellow) believes that there is a pressing need for reform within DEC to address key concerns like systemic oppression and mental health challenges prevalent in academic environments. To ensure credibility of analysis, authors BD and MAC made a conscientious effort to address biases in a transparent manner. This was achieved by openly acknowledging biases, documenting memos, and conducting consensus meetings, in addition to the methods reported below (Birks *et al.*, 2008; Watts and Finkenstaedt-Quinn, 2021). Also, during the interviews, we used informal member checking by summarizing participants' statements back to them to ensure clarity when there was any uncertainty (Bretz, 2008). We believe that these methods enhance the trustworthiness and credibility of the data and analysis, ensuring the findings presented in this paper reflect the data itself rather than our personal perspectives or beliefs.

Participant selection

In accordance with the TCSR model and informed by the survey of doctorate recipients (SDR) (Survey of Doctorate Recipients (SDR) 2021 | NSF - National Science Foundation), our participant selection process focused on recruiting faculty members with diverse personal and contextual identities (Setia, 2016; Lawrie, 2021). This approach aimed to include faculty participants from various geographic locations, university settings, chemical divisions, genders and racial and ethnic backgrounds. To do this, all chemistry doctoral programs across the U.S. were compiled into a list and then grouped into five regions to be sampled proportionally (details can be found in Appendix A in the supplementary information). Faculty emails were gathered from institutional websites of those institutions that were selected randomly within each region, invitations were extended to faculty, and those who expressed interest were invited to share their demographic information and give written informed consent. Initially, interested participants were accepted. However, to ensure representation from a variety of perspectives, as mentioned above, at later stages we intentionally sampled participants from groups which were not well-represented in our sample at that point. Ultimately, our demographic breakdown (see **Figure 1**) shows strong representation across the intended categories. Using the numbers from the SDR as a starting point, we intentionally oversampled certain demographics so that people who hold identities and perspectives that have been minoritized in STEM would be appropriately represented. We excluded one participant from the analysis process because the participant is a teaching faculty who has not trained doctoral students.

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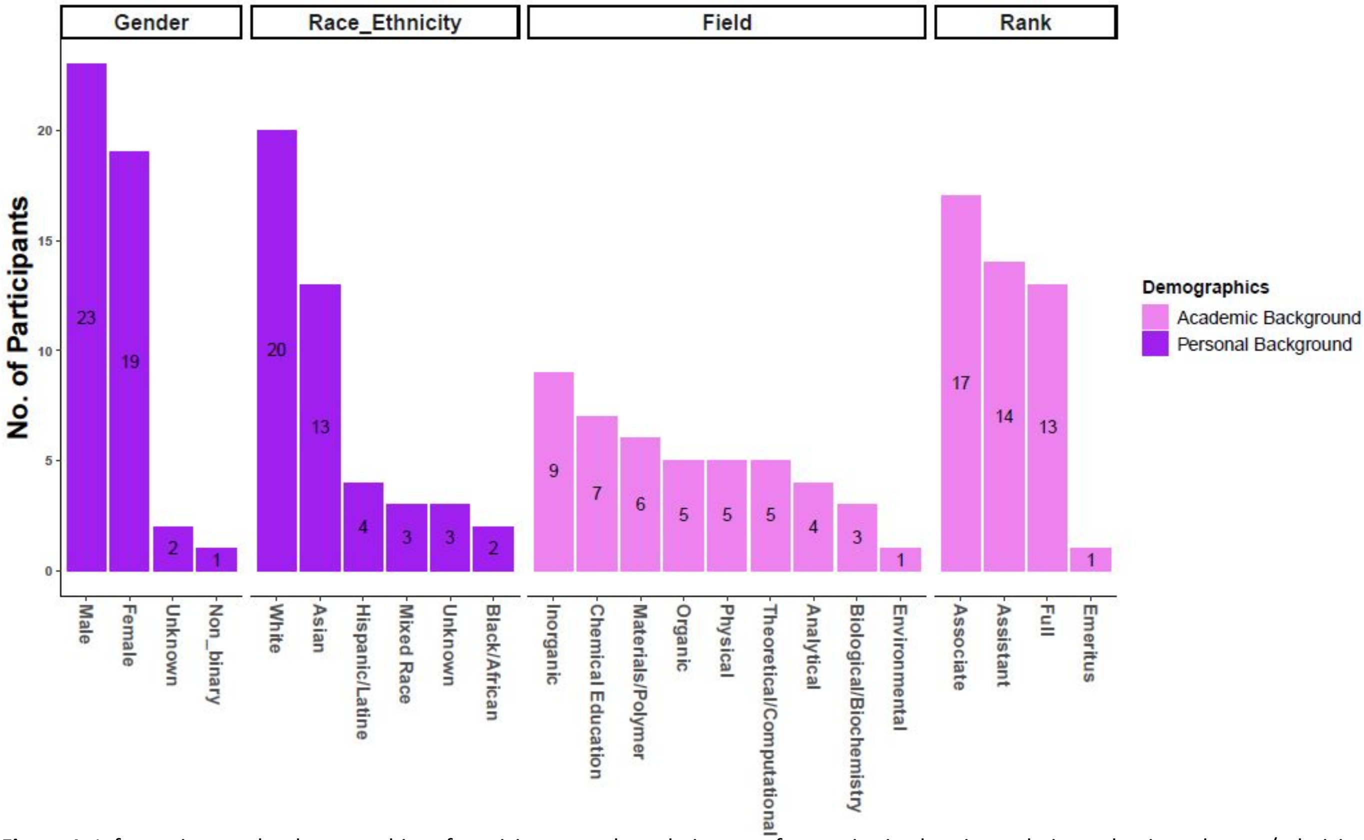

Figure 1. Information on the demographics of participants such as their area of expertise in chemistry, their academic rank, race/ethnicity (with White encompassing individuals of White/Caucasian/European descent), and gender. This information is organized based on decreasing frequency within each demographic category.

* We acknowledge that each participant represents an intersection of all four identity categories: gender, race and ethnicity, field, and rank. To preserve anonymity, we deliberately chose not to display these intersecting identities, as doing so could inadvertently compromise participants' confidentiality.

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Development of interview protocol

The TCSR model was used as a guide to draft the initial interview protocol by authors BD and JH (Woodbury and Gess-Newsome, 2002; Gess-Newsome *et al.*, 2003). Author MAC reviewed the protocol to ensure the framework's constructs were covered. The protocol asks faculty to identify the primary goals of DEC both overarching and for each element of their program together with other contextual and personal questions (more details can be found in Appendix A in the supplementary information).

Codebook development/data analysis

Collaboratively, authors BD and MAC developed the codebook by employing an iterative approach of memoing and consensus-building (Birks *et al.*, 2008; Watts and Finkenstaedt-Quinn, 2021). Analysis was focused on participants' responses to the following questions: "what is the primary goal of [each programmatic element]?", and "what do students actually gain from [each programmatic element]?". NVivo 1.7.1 was used for the initial coding of the goals, and outcomes of the individual programmatic elements. Initially, both authors BD and MAC independently coded the first 18 participant's responses into two deductive codes – one focused on the goal itself and another on what students actually gained. Afterwards, BD and MAC each independently conducted deeper, inductive coding within the overarching codes. Consensus was reached on the deeper codes and their definitions (see **Table S1** in the supplementary information).

Inter-rater reliability

Measures were implemented to ensure reliability of every step in the analysis process. Through inductive coding, authors BD and MAC independently analysed and identified the goals and outcomes of the programmatic elements for the first six transcribed interviews, reaching a complete consensus. Afterwards, both authors independently coded an additional eight participants. Inter-rater reliability (IRR) was calculated for the participants coded by both coders using two IRR metrics, percent agreement (Krippendorff, 2004), and Cohen's kappa (Watts and Finkenstaedt-Quinn, 2021; Rodriguez *et al.*, 2023) and can be found in **Table 1**. The two metrics showed acceptable IRR indicating moderate to high agreement between the coders (Landis and Koch, 1977; Cui and Harshman, 2020). Therefore, the remaining interviews were divided between the coders.

Table 1. Interrater reliability results

Interrater reliability method	Results
Percent agreement	0.955
Cohen's kappa	0.760

Results and discussion

In this study, faculty perspective on the goals and outcomes have been discussed herein. Part I addresses research question 1 and details the goals and outcomes of the programmatic elements, while Part II addresses research question 2 and offers insights into the goals and outcomes of the individual programmatic elements. Part III addresses research question 3 and examines how DEC's primary goals and outcomes align with 21st-century skills identified in the literature for Ph.D. Chemists.

Part I (Research Question 1): From faculty perspective, what are the primary goals and outcomes of the individual programmatic elements of doctoral education in chemistry?

Generally, faculty members articulated goals of the programmatic elements while also acknowledging them as outcomes. However, a few faculty members highlighted specific outcomes that were not mentioned as goals for the elements, while others mentioned goals but did not explicitly identify them as actual outcomes. The details of the goals and outcomes identified by faculty are reported in **Table 2a** and **b** and are discussed below. However, it is important to note that while we report all goals and outcomes identified by faculty, there were several insights that need to be considered as we interpret these results (discussed in *Part II*, below). **Table S2** shows the number of participants that were explicitly asked the questions about the goals and outcomes and the corresponding percentages with respect to the total number of participants interviewed (see **Table S3** for the percentage of participants that were explicitly asked both questions on the goals and outcomes of the individual programmatic elements).

While all faculty-identified goals and outcomes in this study are important, our discussion focuses on the goals and outcomes of the individual programmatic elements where at least 25% of faculty mentioned them. As there were a lot of goals and outcomes to be discussed for each programmatic element, we divided the percentage of faculty that mentioned each goal or outcome into 4 quartiles (75-100 – first quartile, 50-74 – second quartile, 49-25 – third quartile and 1-24 – fourth quartile). It was found that only a few of the goals and outcomes of the individual programmatic elements were in the first and second quartile. Hence the third quartile was chosen as the cut-off point for the goals and outcome to be discussed for each programmatic element. Programmatic elements are discussed based on their average relative importance ranked by faculty participants. We acknowledge the arbitrary nature of establishing these cutoffs in our attempts to communicate results within a reasonable length.

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Table 2a. Percent of faculty with each perspective on the primary goals and outcomes for the individual programmatic elements (first six programmatic elements)

Goals and Outcomes*	Programmatic Elements**											
	Research		Advisor		Publications		Group Mtg.		Candidacy		Coursework	
	G	O	G	O	G	O	G	O	G	O	G	O
Technical Research Skills	68	64	11	4	35	40	6	18	3		24	14
Critical or Independent thinking	59	54	8	13	18	2	24	18	44	19	9	14
Technical Knowledge	43	44	8	9	18	2	35	45	25	13	100	91
Problem-solving skills	36	31	5				3	18	6	13		5
Novel or significant research	34	28		4	24	7						
Communication skills	32	33		4	76	73	65	55	31	25	9	
Career Preparation	30	49	27	22	41	27	6		16	6	12	5
Planning or organizational skills	25	31	5	9	24	33	18		31	31		5
Mentorship	25	8	95	96	12		24	27	3	13		5
Scholarly record	11	15	3		71	27						
Affective outcomes	7	33		9	18	2	6			6		
Networking and Collaboration	7	13	8	17	6	7	56	45	9		3	14
Evaluation and feedback	7	8	19	13	24	2	53	55	56	31	6	
Research resources	5	3	30	26	6							
Teaching skills	5	3	3	4			3					9
Help faculty or department	5		3		12							
Personal resources	2	3	16	13	6							
Ethics	2						3					
Stress or harm mental health			3						3	38		5
Weed Out			3						25	13		
Supplement advisor									3			

Workable environment			14	9			12					
Free food								9				
Advisor Accountability					6							
Advisor or Lab Pairing												
Celebratory fanfare												
Uniform level											26	9

Table 2b. Percent of faculty with each perspective on the primary goals and outcomes for the individual programmatic elements. (continuation of **Table 2a –** next six programmatic elements)

Goals and Outcomes*	**Programmatic Elements****											
	Defense/Diss.		**Lab Rotation**		**Committee**		**Annual Eval.**		**Seminar**		**TAship**	
	G	**O**	**G**	**O**	**G**	**O**	**G**	**O**	**G**	**O**	**G**	**O**
Technical Research Skills			5					8				6
Critical or Independent thinking	22	23					4	8	11	6	9	6
Technical Knowledge	9	23							68	56	38	44
Problem-solving skills								8			3	6
Novel or significant research	22											
Communication skills	75	62					9	23	61	50	47	50
Career Preparation	6		5		17	11	17	8	14	6	31	33
Planning or organizational skills	22	8					9	23	7	13	9	22
Mentorship	3	8	5	8	83	67		23	7	6	19	22
Scholarly record	69	23						8				
Affective outcomes	3	38	5	8			9	8			9	11
Networking and Collaboration	3		15	31	3	11			39	19	9	6
Evaluation and feedback	34	15	1		47	22	87	69	11	13	3	
Research resources								8			25	6
Teaching skills									7		72	33
Help faculty or department	3										44	
Personal resources											53	33
Ethics							4					
Stress or harm mental health	3							8	4	6		
Weed Out												

Supplement advisor			5		73	33	4	8	4			
Workable environment			1	31								
Free food										6		
Advisor Accountability					4	22	17					
Advisor or Lab Pairing			90	100								
Celebratory fanfare	13											
Uniform level												

*These data include all mentioned outcomes, yet some faculty indicated a lack of confidence in these outcomes. Please see Insight III for more details when considering the reported outcomes in this table. The goals and outcomes in this table are sorted by the highest percentage of participants that mentioned the goals and outcomes for **research**. The numbers are the percentages of faculty who responded to the questions "what is the primary goal of the programmatic elements" and "what do students actually gain from the programmatic elements." Each of these percentages have been normalized to the proportion of the number of people that were asked explicitly about these two questions (see **Table S2** for the actual number of participants for each element). The yellow highlights indicate the goals and outcomes discussed in Part I, with the intensity of the colour representing the quartiles: deep colour for the first quartile, medium colour for the second quartile, and light colour for the third quartile.

Legend for abbreviations used for programmatic elements: Group Mtg.– **Group meeting, Candidacy – **Candidacy process**, Defense/Diss.– **Dissertation and Defense**, Committee – **Advisory committee**, Annual Eval. – **Annual evaluation**, TAship – **Teaching assistantship**. The elements are sorted based on faculty rating of their relative importance.

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In the following sections, we do not allude to the fact that statements are from faculty perceptions for succinctness (e.g. “the goal of research is...” versus “faculty perceived the goal of research is...”). Additionally, programmatic elements are formatted in bold while specific codes are formatted in bold/italics for reference.

Research. A similar percentage of faculty participants that mentioned ***technical research skills*** as a primary goal also mentioned it as an outcome of **research**. This skill is highlighted by Participant 1:

“*Well, the research teaches students to do careful experiments and interpret the results from experiments. To modify experiments based on results.*”

To be able to carry out **research**, one needs to first and foremost identify a problem and think about possible ways to solve the problem leading to two primary goals and outcomes mentioned by faculty: ***critical or independent thinking*** and ***problem-solving skills***. However, lacking the necessary foundational knowledge about the **research** to be conducted can make it significantly challenging, if not impossible, to achieve meaningful results. This aligns with the ***technical knowledge*** goal and outcome mentioned by faculty. Faculty participants highlighted ***novel or significant research*** as a primary goal and outcome for **research.** The underlying objective is to facilitate captivating and groundbreaking research that is publishable. This is consistent with a previous study that showed that pursuing a doctoral-level education equips students with the skills needed to excel as innovative researchers (Åkerlind and McAlpine, 2017).

Faculty members emphasize the importance of ***communication skills*** as **research** is contingent upon the proficient communication of its data and results. ***Communication skills*** is one of the six professional development skills needed by STEM students as highlighted in a previous study (Mackiewicz *et al.*, 2023). The overall goal of attaining all these skills is geared towards students’ career path highlighting the reason faculty mentioned ***career preparation*** (St. Clair *et al.*, 2017; Langin, 2019; Okahana, 2019; Cui and Harshman, 2020, 2023; Ganapati and Ritchie, 2021). Through the **research** process, students learn to plan their **research**, design experiments, consider time for completing the research, and prepare documents among others thereby leading to the goal and outcome ***planning or organizational skills***. They also learn to persevere and be persistent as **research** does not always work out with one attempt and they learn to better appreciate the process (***affective outcomes***). Even though it is expected that students would need someone to guide them through the stages of their research (receiving ***mentorship***), it is expected that they would gain ownership of the process along the way. These primary goals and outcomes are also consistent with a report by Casey, a former ACS president (Casey, 2004). The report highlighted the decision by the representative committee in their institution to provide their graduates with specialized expertise in their respective areas, cultivate a broad scientific knowledge base, enhance problem-solving skills, promote the exploration of new challenges, develop strong communication skills, foster teamwork abilities, and instil confidence and independence as scientists. See **Table 2a** for more primary goals and outcomes of research.

Advisor. There is a similarity in the percentage of faculty that mentioned primary goals to those that mentioned outcomes for this programmatic element (see **Table 2a**). Almost all faculty (more than 90% for both goals and outcomes) who participated in this study mentioned ***mentorship***. ***Mentorship*** in this context encompasses guiding the students, giving them advice, serving as a sounding board to them, helping them create research projects, serving as a cheerleader to them, providing them with moral support, mentorship skills, and being accountable for student’s progress among others. The concept of ***mentorship***, as mentioned by the faculty in this study, is viewed from two perspectives. The initial scenario pertains to students receiving mentorship from experts (their advisors or advisory committees) as elaborated by Participant 1:

“*Because they need to learn, and they need someone guiding them as they learn. Since I said that research was so critical that they benefit from having an expert guide them and help identify important research problems. And so that’s one of the main roles of the advisor*”.

The second type of mentorship entails students engaging in mentoring activities or acquiring skills in mentoring others, elaborated by Participant 12:

“……*how to mentor other people, that’s all part of it too. So, it’s a lot that goes into mentoring.*”

Previous studies highlight that research **advisor** is known to be a major contributor to the overall success/progress or failure of a graduate student aside the student’s contribution (Jacks *et al.*, 1983; Trinkner, 2014; Qu and Harshman, 2022). In order for students to thrive in their academic endeavours, it is essential that faculty members provide the necessary components outlined in previous studies (Berelson, 1960; Affero and Abiddin, 2009; Barnes and Austin, 2009; Gardner, 2009). These include, but are not limited to, offering students consistent and valuable feedback regarding their progress, fostering their growth as researchers and professionals, and being readily available for them all of which align with the ***mentorship*** in this study. Serving as a source of additional resources and providing supplementary resources for students (a form of ***mentorship*** found in this study) to enhance their knowledge beyond the scope of their coursework is integral to their development. McLure conducted a study on the impact of advisors on students' academic progress, emphasizing their role as a dependable source of information (McLure, 1989). Mentoring is an important skill that is valuable regardless of the students' chosen career paths. This is because they can potentially be assigned leadership or guidance roles in the future, aligning with ***career preparation***. In this regard, Participant 8 said:

"*But in principle, your advisor, if it's good advisor and there's a good relationship or for some people, if they become role models. So, you may recognize what it takes to be a successful scientist or to be a certain type of scientist, at least a certain type of scientist. And yeah, I think that most has to do with learning and motivation*".

Prior research highlights the importance of mentoring doctoral students to help them explore diverse career paths (St. Clair *et al.*, 2017; Langin, 2019; Okahana, 2019; Ganapati and Ritchie, 2021). An earlier study revealed that support from advisors significantly impact the desire of doctoral students to pursue careers in academia, suggesting that faculty play a key role in students career choice decisions (Seo *et al.*, 2021).

In light ***research resources***, Participant 2 said:

"*Well, first of all, the research advisor will pay the bills. Someone has to write a proposal and get it funded to support the graduate student, right.*"

For students to be able to conduct **research** and while carrying out their duties/responsibilities in chemistry doctoral programs, they need someone to set the stage by providing them with resources (White and Nonnamaker, 2008). Therefore, it is not surprising as faculty mention this as part of the goals of students' having an **advisor**. However, none of the participants indicated whether students aspiring to become faculty members receive training on securing ***research resource***s. Other goals for **advisor** mentioned by faculty can be found in the **Table 2a**.

Publication. The process of preparing and publishing research hones students' ability to communicate complex ideas clearly and effectively (***communication skills***), a vital skill for both academic and non-academic careers. Publications contribute significantly to a student's ***scholarly record***, which is critical for career advancement in academia, research institutions, and industry, where a strong publication record is often a key hiring criterion. Therefore, engaging in the publication process prepares students for future career demands (***career preparation***), teaching them how to navigate peer review, respond to feedback, and meet the rigorous standards of professional research.

Writing and publishing research papers requires a deep understanding of experimental design, data analysis, and the ability to interpret findings (***technical research skills***). These ***technical research skills*** are essential for success in scientific careers. The process of **publication**, from drafting a manuscript to revising and submitting it, demands strong ***planning and organizational skills***. These skills are indispensable in any professional setting, helping students manage projects, meet deadlines, and work efficiently.

Group meeting. Participant 12 acknowledges the value of **group meetings** as a platform for students to practice effective ***communication skills***. It is important for doctoral students to be able to clearly and effectively communicate (oral and written). This includes delivering presentations that convey complex ideas simply and persuasively. Honing these skills enables students to communicate research effectively, engage in academic discussions, and present at conferences, enhancing their scholarly impact and professional growth. This aligns with a previous study showing that group meetings help students prepare for career presentations (Busby and Harshman, 2021).

Some faculty also mentioned ***networking and collaboration*** which in this context encompasses collegiality, networking and collaboration. Participant 14 explore collegiality:

"*It's a chance to learn from other people who are either learning from you or that you're learning from them. It's a chance to have a less formal environment than the classroom to do group learning.*"

Participant 16 highlights networking:

"*they're a place to get various kinds of experts deeply engaged with the people who are closest to you to give you advice about your research.*"

Regarding collaboration, Participant 23 said:

"*…. I want students to collaborate, and so they need to know what other people in the group are doing, and this is a formal way in which they can do that.*"

Building a strong professional network and fostering collaboration with peers, advisors, and industry professionals (when invited to such meetings), are essential for enhancing doctoral students' research opportunities and career prospects. Effective teamwork on research projects and participation in academic communities lead to valuable co-authored publications, presentations, and networking opportunities, addressing concerns from a prior study about the need for chemistry programs to help students connect with non-academic professionals (Cui and Harshman, 2023).

Evaluation and feedback are vital for doctoral students' growth, providing constructive insights on research progress and methodologies. Regular feedback help refine their work, improve research design, and address weaknesses, fostering both robust research and personal development through expert guidance. In light of ***technical knowledge***, Participant 7 highlighted developing effective reading and comprehension skills, understanding key elements in academic texts, and engaging in theory building, as complementary supplement to **coursework**. **Group meetings** serve as a platform for students to learn about the latest tools and methodologies in their field while engaging with advisors and peers to clarify complex concepts and receive practical advice. These sessions also facilitate ***mentorship***, allowing doctoral students to discuss their research, seek feedback, and learn to mentor others, fostering a supportive culture that aids in navigating their academic and professional paths successfully.

Candidacy process. According to our faculty participants, their chemistry programs employ various methods to conduct candidacy exams. These exams are crucial in facilitating the transition of graduate students to the status of a doctoral candidate, which aligns with a previous research (Gordon, 1968). Candidacy process in this study encompass candidacy exams, preliminary, cumulative, comprehensive, or original research proposals. Some chemistry programs do more than one of these exams for candidature. Highlighting ***evaluation and feedback*** Participant 1 said:

"….it evaluates their progress, allows us to provide feedback on their performance…."

During proposal presentation, students must provide thoughtful, well-developed answers to questions, similar to cumulative or candidacy exams. They receive guidance and feedback from their primary **advisor** and **advisory committee**, which offers constructive critiques to refine their proposals and improve their dissertation research. This process helps students address weaknesses, enhance their work, and build confidence while evaluating their skills to determine their readiness to complete the program, aligning with previous study findings (Beebe *et al.*, 1948).

Fostering ***critical and independent thinking*** as highlighted by faculty helps students evaluate literature, develop original research questions, and create innovative solutions. This skill is essential for navigating complex research topics and demonstrates their ability to analyse information and propose novel directions, showcasing readiness for advanced research. Some faculty mentioned ***communication skills*** and Participant 16 expressed it as:

"they know how to speak to different audiences, speak to non-scientists, speak to semi-experts, to undergraduate sophistication and then to their peers."

Effective communication is essential for students during the **candidacy process**, as it enables them to clearly present their research proposals, articulate their ideas and methodologies, and respond to critiques, thereby enhancing their ability to convey their work to diverse audiences (Ananiadou and Claro, 2009). In order to develop a research proposal or successfully complete **candidacy process**, individuals must carefully plan their approach, thus demonstrating their proficiency in ***planning or organizational skills***. ***Technical knowledge*** enables students to understand and apply advanced methodologies and tools in their research field, demonstrating competence in their proposals. Effectively utilizing and explaining these aspects enhances the credibility and feasibility of their work.

There are two goals and outcomes of **candidacy process** that are concerning; ***weed out***, and ***stress or harm mental health***. The "***weed out***" process is designed to assess students' readiness to continue in their doctoral program by ensuring they meet the required academic standards. This aligns with a previous study identifying that some faculty view the candidacy process as a means to weed out students (Nardo, 2024). While it identifies those prepared for advanced research, the process becomes problematic when faculty prioritize filtering out students over helping them succeed. For example, Participant 21 noted that the exams serve as a strict filter, suggesting that students who fail simply lack the necessary ability, rather than focusing on supporting their success. One could have thought that ***stress or harm mental health*** could have been highlighted in terms of managing stress and mental health. However, this was talked about in the negative light of causing ***stress*** for the students as opposed to providing benefits. In this context, Participant 12 stated:

"…just stress and a lost Saturday morning…"

This suggests that some faculty members not only perceive the **candidacy process** as a source of ***stress*** but also as a significant time drain that could otherwise be allocated to more meaningful activities for doctoral students. If this perspective is held by faculty, it raises concerns about the effectiveness of the **candidacy process**. It implies that not all **candidacy processes** are seen as inherently beneficial, indicating a need for a re-evaluation or improvement in its structure to ensure effectiveness.

Coursework. It is not surprising that all the faculty participants mentioned ***technical knowledge*** as the primary goal while 91% of them mentioned it as an outcome. In this study, information pertaining to the field, practical knowledge obtained for conducting research and learning materials to aid in research were classified as ***technical knowledge***. Participant 7 highlighted the primary goal of **coursework** is to equip individuals with the specific knowledge required for their research, offering a deeper understanding than their undergraduate classes, tailored to the analytical needs of their respective projects. This is consistent with a prior study which emphasized the importance of having a strong understanding of the fundamental principles in chemistry for new graduate students to not only succeed but also thrive in the program (Beebe *et al.*, 1948). ***Uniform level*** mentioned by faculty participants was to ensure that all students have a similar level of fundamental knowledge. This is supported by a statement from Participant 4, who highlighted the need to ensure that all students reach the same level in their disciplines within the first year.

Dissertation/Defense. Most faculty mentioned ***communication skills*** as the primary goal and outcome of **dissertation/defense**. The dissertation involves the writing up of research that has been done throughout the doctoral student's training while the defense is communicating it to a general public and/or advisory committee which are all a form of ***communication skills*** expressed by faculty in this study. In addition, some faculty mentioned ***affective outcomes***, ***scholarly record***, ***evaluation and feedback***. This programmatic element helps students gain confidence and appreciation of what they have accomplished (***affective outcomes***) in this period. This is expressed by Participant 13 who highlighted that doctoral students gain a profound appreciation for their accomplishments as they compile a comprehensive view of their work into a book-length presentation, providing them with a lasting and substantial sense of pride and achievement. Also, the work done at the Ph.D. level is mostly expected to be novel, which leaves a permanent record for the students' achievement unveiling the goal and outcome: ***scholarly record***. During the **dissertation/defense** process, students are evaluated and gain constructive feedback (*evaluation and feedback*) that helps them. This is consistent with previous studies which states that dissertation is widely recognized as the ultimate educational output created by its author (Lovitts, Barbara E., 2005), while the oral defense serves as a means to evaluate a candidate's overall proficiency and understanding in their field of study (Frost and Hussey, 1958; Gordon, 1968). See Table 2b for the remaining goals and outcomes of **dissertation/defense**.

Lab rotations. 90% of faculty mentioned that the goals of **lab rotations** is advisor or lab pairing while all of them mentioned it as the outcome. In this regard, Participant 9 said:

"…. and you want to make sure that one, you can get along with them personally."

Lab rotation is a designated period during which students engage with **advisors**, post-docs, and other graduate students across multiple laboratories for specified durations (Barnard and Shultz, 2020; Artiles et al., 2023). This allows them to gain exposure and make informed decisions about which labs they will ultimately join consistent with a previous study (Donkor and Harshman, 2023). Faculty also mentioned ***networking and collaboration***. Participant 46 highlights that by participating in **lab rotation**, students build relationships with senior peers and potential future committee members, gaining valuable connections and resources that benefit them long after joining a lab. This exposure allows students to appreciate and understand various individuals and their unique approaches to work and fosters ***workable environment*** as mentioned by faculty. This is because the lab serves as the focal point for fostering academic and social interactions among lab colleagues, postdocs, and faculty (White and Nonnamaker, 2008).

Advisory committee. Participant 4 highlighted ***mentorship*** saying:

"*the goal in selecting a guidance committee is to select a group of faculty who can help provide a level of expertise, and knowledge, and insight for the project, that will be beneficial to the student.*"

Previous studies indicate that, alongside **advisors**, the doctoral **advisory committee** aids students in planning their proposals, guiding their studies, assisting with dissertation preparation, and conducting final examinations (***evaluation and feedback***), aligning with our findings (Barnes and Austin, 2009; Mauch and Park, 2014). Additionally, the committee provides ***career preparation*** by offering advice and serving as references. Other primary goals and outcomes can be found in **Table 2b.**

Annual evaluation. *Evaluation and feedback* was the most common goal and outcome of **annual evaluation**. Participant 3 said:

"*then the annual evaluation, the semester evaluations that we've had, I think, have been useful in providing feedback and encouragement to the students. And sometimes, you may not tell a student directly how great you think their work is, …*"

The **annual evaluation** is primarily conducted by the student's **advisory committee** which is to provide students with crucial evaluation and feedback on their academic and research progress. These evaluations provide **advisors** and the **advisory committee** a structured opportunity to assess student development, identify strengths, and pinpoint areas for improvement. Constructive feedback helps refine research focus, improve methodologies, and keep students on track with academic milestones, ensuring they meet program expectations while enhancing the quality and impact of their doctoral work. It should also be noted that Participant 35 noted that instead of students actually gaining relationships with other professionals (their advisory committee) during **annual meetings**, they are probably gaining ***stress*** if they have an unsupportive committee.

Seminar/colloquia. Actively engaging in **seminar/colloquia** expand individuals' understanding in a given field while they acquire knowledge regarding the general methodologies employed in specific areas (***technical knowledge***)(Foulk, 1928; Busby and Harshman, 2021). At **seminar/colloquia**, students are expected to present their research findings as well as findings of other people's work found in the literature which delineate ***communication skills*** mentioned by faculty. Additionally, faculty mentioned ***networking and collaboration***. In addition to **group meetings**, **seminar/colloquia** can provide a valuable opportunity for professionals from various fields outside academia to present to students. This would enable students to gain insights into alternative career paths. **Table 2b** contains the additional primary goals and outcomes of **seminar/colloquia**.

Teaching assistantship. From faculty perspectives, **TAship** was seen as the least important despite the goals and outcomes mentioned. Faculty mentioned ***teaching skills*** as a primary goal and outcome of **TAship** where Participant 1 said the goal is to provide doctoral students with experience in teaching scientific material, specifically chemistry. This observation could be attributed to the fact that the majority of responsibilities assigned to teaching assistants revolve around teaching-related tasks (Jepsen *et al.*, 2012). A prior study pointed out that ***teaching skills*** is the most prominent learning goal of **TAship** from the perspective of the graduate student handbook (Donkor and Harshman, 2023). Also, it is one of the 21st-century skills essential for U.S.-trained doctoral chemists in their typical chemistry career roles leading to another goal and outcome: ***career preparation*** (Cui and Harshman, 2020). While some participants argued that ***teaching skills*** are primarily important for those aiming academia, it's important to recognize that nearly every profession requires some level of teaching ability, as emphasized by Participant 3, who noted that regardless of whether individuals go into a corporation, government lab, or academia, the ability to explain concepts clearly is essential. This aligns with previous studies revealed that government scientists and industry professionals both emphasize the importance of this skill in training new employees (Schulze *et al.*, 2014; Cui and Harshman, 2020; Muurlink *et al.*, 2023). To be able to teach, students need to be equipped with specialized knowledge and tools relevant to their field and teaching responsibilities (***technical knowledge***). This proficiency enhances their teaching by allowing them to better support and guide students.

Also, in order to effectively teach, it is essential to possess effective ***communication skills***, highlighting its significance as a goal/outcome aligning with a previous report (National Academies of Sciences, 2018). Also, faculty participants mentioned that the goal of students being teaching assistants is to help in teaching undergraduate courses and labs (not regarded as an outcome by faculty) hence the goal, ***help faculty or department***. This is in alignment with previous studies that emphasized **TAship** roles prioritize institutional needs over providing a high-quality learning experience for graduate students (Austin, 2002; Zotos *et al.*, 2020). Some faculty mentioned that ***personal resources***, such as tuition support and stipends, are essential for alleviating the burden of outside work during doctoral training, as previous research indicates that such employment can impede student progress (Seymour, 2005; Pyhältö *et al.*, 2012). On the other hand, having secure funding ensures that students are provided with the necessary support to focus on their research projects (***research resources***). A previous report highlighted that doctoral programs require students to serve as teaching assistants, aiming to foster educational skills such as pedagogical training and helping undergraduates while also providing them with financial aid aligning with some of the goals/outcomes highlighted by faculty in this study (Golde and Dore, 2001).

Further, the length of this paper is prohibitive of an in-depth discussion for each element about how the TCSR model can shape the goals and outcomes of individual programmatic elements as reported by faculty, However, an example can be used to demonstrate this impact:

The personal factor construct (which includes faculty members' own doctoral experiences) can influence their perceptions of the goals and outcomes of each element. For instance, Participant 33's personal experience as a graduate student shaped their view of the goal of candidacy exam. This is demonstrated by the statement

"… based on my experience as a grad student and my experience at these different institutions, I think the candidacy exam is to show that the candidate is ready to…."

Contextual factors, such as a faculty member's field of interest and area of study, influence the methods they employ and shape their practices (enacted practices). For instance, when Participant 2 was asked what students actually gain from research, the response was:

"…For instance, a chemist have to know a certain technique. So, most chemistry techniques you might learn as an undergrad, but as a solid-state materials chemist, our techniques are not taught typically for undergrads, at the undergraduate level..."

This participant illustrated contextual factor in their response by including the specialized techniques required in their field (solid-state materials chemistry), which are not typically taught at the undergraduate level.

The enacted practices are often the enacted goals that lead to the outcomes of the programmatic elements. For instance, some participants stated that they did not know whether students actually gain the stated goals of the programmatic elements (see Insight III for details). The faculty thinking or perspectives has been elaborated above (Part I) for each of the programmatic elements.

Part II (Research Question 2): What Insights can be drawn from the goals and outcomes of the individual programmatic elements?

Insight one: Misalignment between stated goals/outcomes and enacted practices

The discrepancy between the stated and enacted goals and/or outcomes of the programmatic elements in chemistry doctoral programs, underscores a broader issue of misalignment between stated goals/outcomes and enacted practices (goals and outcomes implemented and students' real experiences or outcomes). For instance, Participant 44 highlighted that the perceived goals of the **dissertation and defense** often differ from the actual practices, suggesting that advisors should better align with the real circumstances rather than adhering strictly to idealized goals.

Participant 35 pointed out that while **seminars** are intended to foster critical thinking and effective presentation, many students find them disengaging, indicating a need for reforms to better meet students' needs. Hence, there should be strategies implemented to increase student engagement in **seminars** by incorporating their input in the seminar structure to address their current needs and enhance their learning experience. This will help maintain their interest and prevent disengagement.

Similarly, Participant 36 noted that the goal of **teaching assistantship** should be to equip students with teaching and mentoring skills, yet many TAs are not given proper training, revealing a gap between intended and actual outcomes.

"Should be providing them with experiences that equip them with the skills to teach and to mentor properly and effectively, students who may not know as much as they do…… So, yeah, our TAs are not taught how to teach, but that should be what they learn at the end of the day."

Participant 46 emphasized that exposing students to teaching through TA roles can uncover latent interests and develop valuable skills, but current practices may not fully support this. These example observations collectively reveal a misalignment between the stated goals/outcomes and the actual experiences (enacted practices) provided by the programmatic elements of various doctoral programs, indicating that the goals and outcomes of some programmatic elements are not effectively realized.

This misalignment is further reflected in participants' responses when asked if the programmatic elements were serving their intended purposes. Some participants affirmed that the elements were meeting their goals, by mentioning the goals of some of the elements, and with a few mentioning periodic evaluations to assess effectiveness. For instance, Participant 4 noted that their program is evaluated every five to seven years, which they believe ensures that the elements align with their goals. However, some participants who affirmed the elements are serving their intended purposes also expressed concerns about a disconnect between the goals and the actual practices. Participant 3, for example, acknowledged the stated goals of some elements but pointed out that sometimes there is a disconnect between some programmatic elements. Participant 23 acknowledged that while the system's elements serve their intended purposes, it is imperfect, especially in terms of the timing for students' readiness to propose and defend original ideas as students may not be ready to propose and defend original ideas. Other participants said the elements were not serving their intended purposes and pointed out problems with some programmatic elements. In that light, Participant 14 highlighted specific issues, such as **coursework** being overly broad, **annual meetings** requiring tweaks to be more effective, and **seminars** being considered time-wasting activities that could be replaced with more useful alternatives. These differing perspectives reveal a misalignment between the program's stated goals and how the programmatic elements are enacted in practice.

Insight Two: Problematic Structure of the Programmatic Elements

Our results reveal that the structure of the programmatic elements in US chemistry doctoral programs often fails to align with students' needs, leading to stress, frustration, and a diminished educational experience. For example, Participant 30 acknowledged the ***stress*** induced by **coursework** and described the **candidacy process** as *"exist to torture students psychologically."* Participant 3 identified the **candidacy process** as a major source of ***stress*** that diminishes its perceived importance, while Participant 24 viewed it as a mere hurdle rather than a preparation tool.

Participants highlighted that rigid structures and misalignment among programmatic elements undermine their effectiveness and intended purposes, suggesting a need for reform. For instance, Participant 24 indicated that **coursework** is most useful when closely connected to students' research projects, suggesting that the lack of such alignment makes other programmatic elements less effective. Participant 23 echoed this sentiment, finding **coursework** frequently unhelpful due to its lack of synergy with **research**.

"......I'll be honest, I don't think coursework in graduate school is super helpful because it depends on, I guess, what your research is. But oftentimes your research may not be synergistic with the courses that you take. And so sometimes it feels like you're doing all this work for courses for things that you may never use......"

Participants also discussed specific issues with the programmatic elements. Participant 33 pointed out that the effectiveness of **coursework** depends on its structure, with well-structured courses being beneficial and poorly structured ones feeling irrelevant, while Participant 24 emphasized that the effectiveness of **lab rotations** depends on their structure. Participant 31 criticized the training for teaching assistants as insufficient for developing pedagogical skills, suggesting a need for better-focused training programs. The mention of *"cheap labor"* by this participant hints at an underlying concern about the use of **TAship** as a cost-effective resource rather than investing in students' development as educators. This reflects a broader issue where the role of TAs might be undervalued in terms of their professional growth.

Participant 32 questioned the value of the **dissertation and defense**, proposing that they could be eliminated as they often fail to provide formative experiences for students. Participant 33 stated that for **dissertation and defense**, students gain confidence (outcome) but there is no way to assess this.

Additionally, the issue of uneven advising was noted, with some faculty not able to provide effective mentorship, which can hinder students' success, consistent with previous studies (Austin and McDaniels, 2006; Golde and Walker, 2006; Barnes and Austin, 2009). While this study does not identify the cause of this, participants noted that it may not necessarily be the advisors "fault," but that a variety of factors can contribute to ineffective mentorship. This is in line with previous studies that have shown poor **advisor** relationships such as inadequate mentorship, mismatched expectations and poor communication between advisors and students, and power imbalance contribute significantly to doctoral program attrition (Jacks *et al.*, 1983; Barnes *et al.*, 2011, 2012). It is crucial for faculty and program administrators to address these issues and ensure that the structure, goals and outcomes of programmatic elements are effectively implemented and aligned with program goals and students' needs.

Insight Three: Lack of Certainty of Programmatic Elements' Goals and Outcomes

Participants frequently expressed uncertainty about benefits being derived from the programmatic elements in chemistry doctoral programs. This is similar to a previous study's finding where faculty expressed levels of uncertainty in communicating the goals of chemistry doctoral programs (Donkor *et al.*, 2024). For example, Participant 30 admitted,

"I have no idea. I don't even remember what I got out of it." when asked about the **candidacy process**, while Participant 12 humorously questioned its purpose, saying,

"Man, I don't know. I'm okay if those disappeared."

Similarly, Participant 24 doubted the value of writing a **dissertation**, asking,

"Why on earth do we make people write a book that nobody reads?"

Participants 20 and 21 were confused about the purpose of **lab rotations**, with Participant 20 stating,

"I don't know why they set it up in the first place…"

Participant 31 criticized the effectiveness of **teaching assistantship**, saying,

"Cheap labour. I don't know. Oh yeah, so it is help them to be able to teach better, but I'm not certain that the way the general TAship here is going to help that much with it. I mean, I guess it makes you a little bit more comfortable talking at students, but I don't know that you learn a lot about pedagogy or anything like that. So yeah, I don't know."

It is unclear how many of the outcomes indicated by faculty align more with faculty "hopes" or "assumptions" as opposed to actual outcomes. Often participants acknowledged that there was no real way to assess the outcomes. For example, Participant 41 said,

"…we hope they actually gain the knowledge…"

When asked what students actually gain from **coursework**, indicating a lack of real evidence supporting these aspirations. Thus, it is unclear how many of the outcomes are actual outcomes.

Participant 24 also expressed uncertainty about whether the programmatic elements are achieving their intended goals by indicating that we as researchers may be wrong in assuming that the programmatic elements have intended goals. This participant shared an anecdote about a faculty meeting in which the purpose of **coursework** was questioned, but there was no apparent answer given by the faculty. The participant recalled that a colleague stated that courses are "performative" and only necessary to maintain accreditation, while another proposed that courses should align with the specific activities of researchers, suggesting a need for more information about lab work to choose relevant courses. Participant 24 summed up the uncertainty by stating:

"And the fact that we were having this question about what is the point of these courses, and we really weren't super sure indicates to me that there really may not be an intended purpose for those courses beyond it's a thing we've always done."

These responses reflect a broader issue: a significant lack of certainty regarding the goals and outcomes of the programmatic elements. The uncertainty expressed by faculty suggests that the goals and outcomes of these elements are not effectively communicated, leading to confusion, a perceived lack of value, and potentially hindering the effective achievement of program goals. These findings highlight the need for better alignment and clearer communication of the goals and outcomes of these programmatic elements to enhance their effectiveness and relevance in doctoral education in chemistry.

Part III (Research Question 3): How well do these goals and outcomes align with the reported overall goal (preparing students for careers)?

In order to determine the extent to which the goals and outcomes of the individual elements are in alignment with the overall goal of doctoral education (preparing students for their careers (Donkor *et al.*, 2024)), the codebook was compared to existing literature addressing skills needed for sciences and/or chemists in the 21st-century. Two main resources were combined for a robust assessment of what documented skills or outcomes are needed for modern career preparation in DEC. Initially the National Research Council's (NRC) 21st-century skills were considered as an authoritative resource on skills necessary for success in education and careers (National Research Council, 2012). These 21st-century skills are broadly categorized as eight clusters of skills within three overarching areas of competency (inter-personal, intra-personal, and cognitive as shown in **Figure 2**). Though there was good alignment of this categorization with our codebook, the categories were considered too broad to adequately answer our research question. For a more context-specific approach, the 21st-century skills clusters from the NRC report were then compared with the twelve workforce skills necessary for chemistry careers identified by Cui and Harshman (Cui and Harshman, 2020). These twelve skills clearly aligned with and expanded upon six of the eight skill clusters identified from the NRC report, with representation in each of the three overarching competency areas. Each coder (BD and MAC) then compared the twelve skills from Cui & Harshman with the existing codebook, and nine codes were found to be represented almost exactly in the name of the code and the definition identified by BD and MAC (full definitions can be found in **Table S1** of the supplementary information) with the remaining three found to be represented, at least in part, by other codes. In addition, the codebook skills were compared to the NRC 21st-century skills cluster, and it was found that the "Creativity" cluster was represented in our codebook, though it was not identified by Cui & Harshman. Based on these findings the twelve skills identified by Cui & Harshman was expanded to include creativity, giving thirteen 21st-century skills needed for professional chemists (**Figure 2**). The clear alignment between these two sources and our codebook lends credibility to our analysis and gives a framework to use when answering Research Question 3.

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	21st Century Skills Cluster (National Research Council, 2012)	Cui & Harshman Skills for Chemists (Cui and Harshman, 2020)	21st century skills needed for professional chemists	Codebook Skills
Cognitive Competencies	Cognitive processes and strategies	Planning and organizational skills Problem solving Critical thinking	Planning and organizational skills Problem solving Critical thinking	Planning or organizational skills Problem solving Critical or independent thinking
	Knowledge	Technical knowledge	Technical Knowledge	Technical Knowledge; Technical research skills
	Creativity	N/A	Creativity	Novel or significant research
Inter-Personal Competencies	Intellectual openness	N/A	N/A	N/A
	Work ethic/conscientiousness	Organizational awareness	Ethics & Organizational awareness	Career Preparation**; Ethics **
	Positive core self-evaluation	Personal value/attributes Personal growth/development	Personal value/attributes Personal growth/development	Affective outcomes** Mentorship (receiving); Evaluation and feedback**
Intra-Personal Competencies	Teamwork and collaboration	Teamwork/collaboration Networking skill	Teamwork/collaboration Networking skill	Networking/collaboration
	Leadership	Teaching skill Management skill Communication skill	Teaching skill Management skill Communication skill	Teaching skills Mentorship (learning how to mentor) Communication skills

Figure 2. An overview of the alignment of the skills framework used to assess career preparation in DEC. First column: 21st-century skills categorized by the National Research Council (National Research Council, 2012); Second column: skills for professional chemists identified by Cui & Harshman (Cui and Harshman, 2020); Third Column: The combination of these used to assess career preparation in DEC (21st-century skills needed for professional chemists); Fourth Column: Skills identified in this study as goals and/or outcomes of programmatic elements of DEC. Not included in this were non-skill codes and outcomes, or those found to be specific to graduate training rather than career preparation (e.g. advisor selection, or helping department)

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To answer the research question, the goals and outcomes identified for each programmatic element in this study were then compared to the thirteen 21st-century skills needed for professional chemist identified in literature as shown in **Table 3** (National Research Council, 2012; Cui and Harshman, 2020). Generally, all the programmatic elements contribute to these skills, indicating that the goals and outcomes of the programmatic elements are well-aligned with the intended goal of chemistry doctoral education. However, comments made by several participants make it clear that although the goals of these elements may be intended to prepare students for their career, faculty are hesitant to vouch for actual outcomes, making the degree of alignment of *outcomes* questionable (see Insights I, II, and III above). Faculty perspectives indicate that the integration might lack depth, practical application, or true effectiveness. Without developing evaluation for the effectiveness of these outcomes, it is unclear how much of this is what the faculty "hopes for" with no real evidence, as noted above in Insight III. For instance, looking deeper into ***career preparation*** in **Table 3**, first glance indicates that there are intended goals and actual outcomes that prepare students for their career within every programmatic element, yet there is evidence that a student aspiring to become a research-intensive faculty may not receive sufficient training or guidance on critical skills such as teaching and mentoring students (Committee on Professional Training, 2015; Heemstra and Moore, 2021; Deng *et al.*, 2024), setting up a lab, and securing funding among others. This is supported by a statement by Participant 8:

"I didn't receive any training and mentorship in my life. I have never been trained to be a mentor. So, in that sense, very likely I am not very good in many areas because again, I have been guided by my own gut of what to do. And when you are guided by your own gut, I think that you just do things that fit with your own persona and that doesn't necessarily get the most appropriate for everybody's personas."

Furthermore, this issue is compounded by the fact that many doctoral programs focus heavily on academic preparation, even as the career aspirations of graduates increasingly extend beyond academia, often leaving them underprepared for non-academic careers (Golde and Dore, 2001; Donkor *et al.*, 2024). This is elaborated by Participant 40 who cited that candidacy exams could be more effective if they provided tailored feedback to help students align their current focus with their future career goals, such as highlighting overlooked skills like budgeting or stakeholder management for those aiming to work in nonprofits.

Ultimately, despite faculty mentioning that most of the elements had goals/outcomes related to ***career preparation***, these important concerns still exist.

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Table 3. Alignment of DEC primary goals and outcomes with literature identified 21st-century skills necessary for Career Chemists.

21st-Century Skills for Professional Chemists Goal (G) Outcome (O)*	Programmatic Elements											
	RS	AD	PB	GM	CE	CW	DD	LR	AC	AE	SM	TA
Communication skills												
G	✓	✓	✓	✓	✓	✓	✓	×	×	✓	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	×	×	✓	✓	✓
Critical or independent thinking												
G	✓	✓	✓	✓	✓	✓	✓	×	×	✓	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	×	×	✓	✓	✓
Mentorship (learning and receiving)												
G	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Networking/ Collaboration												
G	✓	✓	✓	✓	✓	✓	✓	✓	✓	×	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	✓	✓	×	✓	✓
Novel or significant research												
G	✓	×	✓	×	×	×	✓	×	×	×	×	×
O	✓	✓	✓	×	×	×	×	×	×	×	×	×
Planning or organizational skills												
G	✓	✓	✓	✓	✓	✓	✓	×	×	✓	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	×	×	✓	✓	✓
Problem solving												

G	✓	✓	×	✓	✓	✓	×	×	×	✓	×	✓
O	✓	✓	×	✓	✓	✓	×	×	×	✓	×	✓
Teaching skills												
G	✓	✓	×	✓	×	✓	×	×	×	×	✓	✓
O	✓	✓	×	✓	×	✓	×	×	×	×	✓	✓
Technical knowledge/research skills												
G	✓	✓	✓	✓	✓	✓	✓	✓	×	✓	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	✓	×	✓	✓	✓
Affective outcomes***												
G	✓	✓	✓	✓	✓	×	✓	✓	×	✓	×	✓
O	✓	✓	✓	✓	✓	×	✓	✓	×	✓	×	✓
Evaluation***												
G	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Career preparation***												
G	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
O	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Ethics***												
G	✓	×	×	✓	×	×	×	×	×	✓	×	×
O	×	×	×	×	×	×	×	×	×	×	×	×

NB: 21st-century skills without *** are skills that align perfectly with the literature identified 21st-century skills necessary for Ph.D. Chemists while those with *** do align partially with the literature identified 21st-century skills necessary for Ph.D. Chemists.

(✓) means at least one participant mentioned it as a goal/outcome for the programmatic element.

* These data include all mentioned outcomes, yet some faculty indicated a lack of confidence in these outcomes. Please see Insight III for more details when considering the reported outcomes in this table.

RS – **Research, AD – **Advisor**, PB – **Publications**, GM – **Group meeting**, CE – **Candidacy process**, CW – **Coursework**, DD – **Dissertation and Defense**, LR – **Lab rotations**, AC – **Advisory committee**, AE – **Annual evaluation**, SM - **Seminar**, TA – **Teaching assistantship**.

ARTICLE

Conclusions and implications

Generally, twenty-seven goals and outcomes were identified for the programmatic elements based on faculty perspectives, reflecting a range of goals and outcomes within the doctoral program. Faculty members outlined specific aims for various elements of the program and provided a framework for understanding the intended contributions of each programmatic element to students' academic and professional development as well as the program's overarching goal.

The examination of the goals and outcomes of the programmatic elements of chemistry doctoral programs yielded three key insights:

First, there is a misalignment between stated goals and enacted practices, highlighting the need for reform to enhance program effectiveness. Educating doctoral students requires more than just addressing the programmatic elements in isolation; it demands a holistic approach where each programmatic element, from research to teaching assistantship, aligns with the overarching program goals (preparing students to be competitive for various careers). Reforms should focus on improving the communication and integration of programmatic elements' goals and outcomes and providing practical training that reflects real-world applications. If there is misalignment, students' educational experiences and professional growth can be diminished and/or hindered. To better support students, programs must align elements' goals and outcomes with their program's goals, ensure clear communication of goals and outcomes, and adapt based on student feedback and evolving standards. This misalignment has broader implications for all stakeholders: students may miss key opportunities for growth, faculty may struggle to mentor effectively, administrators must address gaps to improve program coherence, and funding agencies should support initiatives that align program goals with outcomes to enhance the quality of doctoral education.

Second, there are significant issues in the structure of chemistry doctoral programs, emphasizing the need for reform and better alignment of programmatic elements. Structural misalignment between the programmatic elements contributes to student stress, frustration, and diminished educational value. These challenges underscore the importance of integrating programmatic elements to support students' research and professional development. Uneven advising quality and inadequate training for teaching assistants further compound these issues. To improve program effectiveness, faculty and administrators must address these issues by enhancing communication, alignment, and support systems. Faculty should offer more relevant **coursework** and mentorship, while administrators should restructure programs to align with students' research goals and professional needs. The problematic structure of the programmatic elements undermines both academic and professional growth of students. Therefore, faculty and administrators should make efforts to address these issues, while funding agencies should support initiatives that prioritize the creation of student-centred, well-structured doctoral programs to improve educational outcomes.

Third, there is uncertainty about the benefits derived from the key programmatic elements in chemistry doctoral programs. Faculty perspectives reveal that the goals and outcomes of programmatic elements such as **coursework**, **candidacy process**, and **lab rotations** among others are unclear. This lack of clarity can result in misaligned goals/outcomes and ineffective education for students. To address these issues, faculty and program administrators must clearly articulate the goals and outcomes of each programmatic element, ideally including them in written documents to ensure alignment with program goals and student needs. This will enhance program coherence, improve the doctoral education experience, and benefit all stakeholders. For students, clearer goals will reduce confusion and frustration, while faculty will be better equipped to support student learning. Also, administrators should ensure that programmatic elements are beneficial and relevant.

The study also indicates that while the structure of chemistry doctoral program is designed to incorporate essential 21st-century skills to prepare chemists for their careers, the actual integration of these skills is questionable. The alignment between programmatic goals/outcomes and workforce needs exists at a conceptual level but may fall short in practice. Faculty acknowledge that 21st-century skills needed for career chemists like ***communication skills***, ***networking and collaboration***, and ***career preparation*** among others are theoretically included in the program, yet the depth, practical application, and acquisition of these skills may be limited. This suggests a need for assessment (and potentially reform) to ensure that these skills are not only addressed in theory in the program's curriculum but are genuinely developed and effectively integrated into students' educational experiences, thereby enhancing their readiness for real-world careers.

To implement change reflective of these key insights, program advisors can encourage their faculty to engage with self-reflection questions, as outlined in Table 2 of Harshman's review of doctoral education in chemistry (Harshman, 2021). This will allow faculty to critically evaluate how well these skills are being incorporated and to identify areas for improvement in their teaching and mentoring practices and program structure.

Also, programs with clearly defined goals of the program and their programmatic elements can determine how to best align enacted practices with those goals (Donkor and Harshman, 2023). To support this, written documentation of goals and outcomes of each programmatic element, paired with regular evaluation and feedback, would enhance clarity and ensure that programs' goals are explicit and actionable. Regularly collecting feedback from students and faculty through surveys or focus groups would be essential for identifying and addressing misalignments, helping to ensure that programmatic elements meet student needs and broader program goals. Furthermore, fostering open communication among students, faculty, and administrators creates additional opportunities to identify areas for improvement and implement solutions.

Although this paper offers insights into the structure and effectiveness of doctoral programs in the United States, the implications extend beyond this context, offering contributions that can resonate internationally, given the commonalities of graduate education worldwide. While the study centres on chemistry doctoral programs, the findings regarding misalignments between stated goals and enacted practices, structural deficiencies, and unclear outcomes are widely applicable to doctoral programs in other disciplines and countries. By advocating for a holistic, student-centred approach to curriculum design, clear articulation of goals, and meaningful integration of professional development elements, this paper offers a framework that can be adapted to a variety of educational contexts. Consequently, its outcomes contribute to a broader understanding of how to enhance the effectiveness and relevance of doctoral programs, ensuring they better meet both academic and professional needs of students globally.

Limitations

Due to the fact that there are many programmatic elements in DEC, we could not cover all the twelve programmatic elements in a single session of interview with participants. We addressed a minimum of three and a maximum of eight programmatic elements with participants respectively due to time constraints. Some participants chose to extend their time beyond the stipulated interview timeframe, while others chose not to, resulting in variations in the number of elements covered. It is important to consider this limitation when interpreting the research findings in this study. Also, faculty members who participated in this study did so voluntarily, bringing specific perspectives and experiences. It is important to note that their perspectives may differ from those who chose not to participate, potentially introducing bias. While our study may not comprehensively capture the full spectrum of faculty perspectives, this is a common challenge in both qualitative and quantitative research. To combat this, we aimed to ensure a representative sample, we randomly sampled faculty from diverse chemistry doctoral programs, considering their academic (rank and primary area of interest) and personal (gender and race) demographics.

Author contributions

Author's BD and MAC were involved in all CRediT roles but Funding acquisition while JH was involved in Conceptualization, Funding acquisition, Methodology, Project Administration, Supervision, and Writing - reviewing and editing.

Conflicts of interest

The authors declare no competing financial interest.

Data availability

Per the IRB approval process, interview transcripts and resulting analyses are not made publicly available.

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Ethical Considerations

This paper has followed the ethical guidelines for human subject's research in line with the approved IRB (Auburn University) for this study.

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Supplementary Information

Doctoral Education in Chemistry: Faculty perspectives on programmatic elements' goals and outcomes

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Contents

Goals and Outcomes Tables

Table S1. Codebook on the codes and definition to the primary goals and outcomes of the individual programmatic elements.

Code	Description
Goals of Elements	Describing goals of individual elements, i.e. responses to what is the goal of the individual programmatic elements.
Goal itself	Responses to "what is/are the goals of the individual programmatic elements?"
Actually get	Responses to "what do students actually gain from the individual programmatic elements?"
Advisor accountability	Keep the advisor from negatively harming students, provide checks and balances on their power over students, extra set of eyes watching, they become your defense against the dark arts, vouch for them
Advisor or Lab pairing	Exposure to a PI before they actually join a research group, allow students to get exposure to a different people, different potential mentors, select an advisor, or the advisor chooses a student, the advisor gets a chance to see the students.
Affective outcomes	To gain an appreciation, confidence, emotional growth, satisfaction, self-confidence and pride, excitement, empathy (they will judge professors less harshly because they themselves are being judged at the same time), get happy, motivate them, interest, gains understanding of what effort it takes to produce and validate new results, persistence, perseverance, resilience, recognition, not to be ashamed of my accent
Career preparation	Preparation for their career, develop a career, essential skill for employment, serve the vocational skill, training students so that they will have options, mentoring students into teaching careers, develop skills and knowledge and abilities and ways of reasoning that would be productive in their careers, it prepares for a huge variety of career path, put on their CV to get an academic job, get the experience that they can put on a resume, getting a letter of recommendation, need other references
Celebratory fanfare	Celebration, fanfare

Communication skills	Communication, being able to write, to be able to summarize the work, to put all research together, present work, the ability to converse on a topic at a high level, giving presentations, practice talks, speaking at a public lecture, discuss research, oral talk, outreach opportunities (science communication, more informal)
Critical or Independent thinking	Contributing their own ideas, think independently, able to synthesize this information together, independent thought, to develop their critical thinking skills, think for themselves, answer questions from curious people, they have to be able to not just doing experiment but what does it mean and what does it mean to have next steps and what can you propose to advance the area, to critique papers, develop independence in research, grow on their own, taking more ownership of the project and contributing their own ideas, feel a sense of ownership of the project, independent scientist, lead projects later on, you learn things well when you teach it, self-learners
Ethics	Discus ethical issue, discussion on general ethical issue, train them in rigor and ethics in doing research
Evaluation and feedback	Evaluation, get feedback, to keep the student on track, review everything that they've accomplished, self-reflection. Communicating expectations to the student.
Free food	Free food
Help faculty or department	They can get tenure, to help their (faculty) own research succeeds, to help the undergraduates, make our jobs sort of easier at the university, cheap labor, to save money, make sure NSF and NIH and other agencies are happy.
Technical knowledge	To gain a body of knowledge, to know the status of the field, the language of the field, to lay the foundation of knowledge, breadth of knowledge, foundational and fundamental chemical knowledge, knowledge base, depth of knowledge, technical knowledge, searching the literature for assistance in either designing experiments, get exposed to science outside of

		their specific research interests, to expose them to other people's work, expertise-deep grounding of own area of research,
	Mentorship	Mentor, mentoring skill, mentorship, guiding them as they learn, help the student, give direction, guides them, gain the advice and support, some level a cheerleader, moral support, become role models, having them there as a sounding board, venting off frustrations, maybe within mentorship, but someone/a committee who is primarily responsible for the students' progress, someone that's held accountable for all this stuff. If it mentions specific skills for them to learn we put that in the other goals codes
	Networking and Collaboration	Interconnect with each other, to know what everybody in the lab are doing, to learn from other people, to get various kinds of experts deeply engaged, to get exposure to a different people, collegiality, be able to mitigate people disgruntle, to work with the other students in the lab, how different people's projects interconnect with each other, if collaborations are specifically mentioned, establishing collaborations, interdisciplinary teams, Working with others
	Novel or significant research	New knowledge they've developed as a result of their efforts, proposing new ones, developing new technologies, creating new knowledge, co-inventor, developing a new methodology or developing a new different technique, creating new knowledge, formulate new ideas and concepts on the fly, engaging in creative activities, to make their own mark on science, very high-impact work. Move an area forward, push the limits of science.
	Personal resources	Funding, money, stipend, salary, pay tuition
	Planning or organizational skills	Organizational skills, prepare themselves and documents, plans for the completion of their Ph.D., they're organizing a seminar, planning, developing, or designing an experiment, time management skill, learn some structure from that, multitasking
	Problem-solving skills	To solve problems, solve problems, problem solving skills, address some gap, to address scientific questions

Research resources	Support of extramural funding that is required to make the research go, space for research, funding, funding for research
Scholarly record	It leaves a permanent record of the work, serves the function of providing tangible evidence, it puts a nice bow on it, Ph.D. level research document, getting publications.
Stress or harm mental health	Just stress and a lost Saturday morning, torture students psychologically, students see it as a hurdle
Supplement advisor	add secondary kind of research advice for what they're doing, get second opinion about their research
Teaching skills	To give them experience in teaching, learn how to teach, to explain to somebody else, and teaching oneself, independent learner
Technical research skills	Formulating or defining a problem, designing experiments, executing experiments, interpreting experiments, pivoting or revising experiments based on outcomes, identifying patterns, identifying new strategies, having students do research, to engage in research, discover how slowly things go in some fields and how fast in other fields activity, Interpret the data, gain practical experience. "How science is done" -counts for Research. If they are talking from mentor perspective, it is mentorship.
Uniform level	To bring them up to a uniform level across the cohort, harmonize everybody's background, fill in gaps from their undergraduate education
Weed Out	to remove bad students, like a weeding out, to ensure some quality control in the people that make it to the end of our program, checkpoint for ensuring that they're going to meet that standard
Workable environment	Advisors create an environment where it's a good learning environment, a good lab environment, build a team and make it work, whether they feel comfortable in a group or lab. Not creating an opportunity for research necessarily but creating a positive environment.

Table S2. Number of faculty who responded to "goal – what is the primary goal of the programmatic elements" and "outcome – what do students actually gain from the programmatic elements" along with the respective percentage to the total number of participants interviewed.

Programmatic Elements	Goals	Percentage out of the 45 Participants (%Goals)	Outcomes	Percentage out of the 45 Participants (%Outcomes)
Advisor	37	82.22	23	51.11
Advisory Committee	30	66.67	9	20.00
Annual Evaluation	23	51.11	13	28.89
Candidacy Process	32	71.11	16	35.56
Coursework	34	75.56	22	48. 89
Dissertation and Defense	32	71.11	13	28. 89
Group meetings	34	75.56	11	24.44
Lab rotation	20	44.44	13	28.89
Publication	17	37.78	15	33.33
Research	44	97.78	39	86.67
Seminar	28	62.22	16	35.56
Teaching Assistantship	32	71.11	18	40.00

Table S3. Faculty that were explicitly asked about both the primary goals and outcomes of the individual programmatic elements.

Goals and Outcomes	**Programmatic Elements**											
	RS (39)	**AD (23)**	**PB (15)**	**GM (11)**	**CE (16)**	**CW (22)**	**DD (13)**	**LR (13)**	**AC (9)**	**AE (13)**	**SM (16)**	**TA (18)**
Technical Research Skills	46		13			14						6
Critical or Independent thinking	38	4	7	9	19					8		6
Technical Knowledge	21	4	7	36	6	86	8				50	28
Novel or significant research	21	4										
Communication skills	18		60	36	19		46			8	50	33
Career Preparation	15	9	27			5			11	8		17
Planning or organizational skills	13		13		13		8				6	6
Problem-solving skills	10			9	6							6
Mentorship	5	91		18					67	23	6	11
Personal resources	3	13										33
Research resources	3	26										6
Networking and Collaboration	3	4		18							13	
Scholarly record	3		20				8					
Teaching skills		4										28
Affective outcomes										8		6
Evaluation and feedback		4	7	45	19		8		22	69	6	
Stress or harm mental health					6						6	
Supplement advisor		4							33			
Advisor Accountability									22			
Advisor or Lab Pairing								100				
Workable environment		4						8				
Uniform level						5						
Celabratory fanfare												
Ethics												
Free food												
Help faculty or department												
Weed Out												

* The goals and outcomes in this table is sorted by the highest percentage of participants that mentioned same goals and outcomes for **research**. Numbers are the percentages of faculty who responded to both questions rounded to the nearest whole number.
RS – **Research, AD – **Advisor**, PB – **Publications**, GM – **Group meeting**, CE – **Candidacy process**, CW – **Coursework**, DD – **Dissertation and Defense**, LR – **Lab rotations**, AC – **Advisory committee**, AE – **Annual evaluation**, SM - **Seminar**, TA – **Teaching assistantship**. The elements are sorted based on faculty rating of their relative importance. The numbers in () represents the total number of faculty explicitly asked both questions.

Appendix A. Method (additional)

Development of Interview protocol

In the first round, BD and MAC conducted interviews with a cohort of 7 participants. Subsequently, an interim halt was introduced in the interview process to facilitate the development of a codebook and to identify any necessary refinements to the interview protocol. Following an initial analysis of these 7 interviews, minor adjustments were made to the interview protocol, involving the reordering of certain questions and enhancing question clarity. For the second round of interviews, involving 12 participants, BD and MAC employed the refined interview protocol. The interview was paused, and data analyzed. The interview protocol was adjusted to prioritize the discussion of programmatic elements that had received comparatively less attention, positioning them at the onset of the interview for the remaining interviews. Notably, programmatic element, research was addressed first, irrespective of the number of participants who had previously discussed it, given its status as the most pivotal programmatic element.

Codebook Development/Data Analysis

Codes similar in definition were combined. For example, the mentorship code encompasses two different types of mentorship. The initial one is students receiving mentorship (where faculty are guiding, mentoring, advising or helping students) while the second is students giving mentorship (where faculty train students to become mentors). However, these two codes were combined as they were all forms of mentorship. Other codes combined were collegiality and networking which were all combined into the networking code. The collegiality code comprised of collegiality, working with other students in the lab, being able to mitigate people disgruntle, etc. while networking was more of interacting with others (colleagues or professors), and getting exposed to other people. The two codes were similar in the sense that they were about students interacting in one way or the other with people inside and outside of their field, hence, combined.

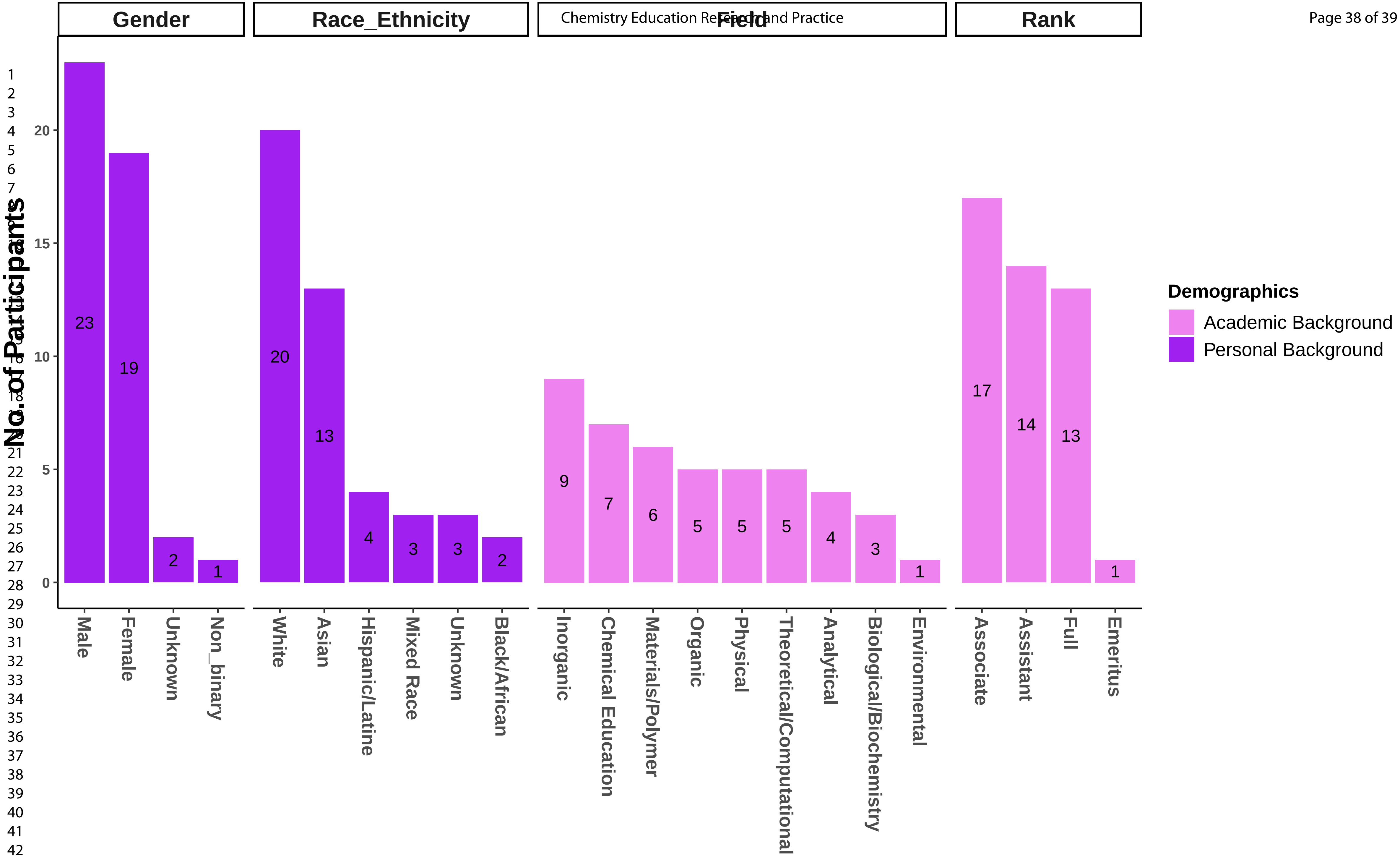
In comparison of the goals and outcomes identified in this study to literature, we identified 12 workforce skills; nine were found to be represented almost exactly in the name of the code and the definition identified by BD and MAC and the remaining three were found to be represented, at least in part, by other codes. For instance, personal attributes from the previous study[11] were partially covered by affective outcomes in this study, while collaboration skills and networking were combined in our study. Management skills in the previous study aligned more with the mentorship component, where students learn to mentor others (in our study). The personal growth and development of the previous study better aligned with aspects of our evaluation and feedback, along with some part of critical or independent thinking (becoming independent part). Organizational awareness aligned with the career preparation and ethics in this study. Therefore, we replaced these skills with corresponding goals and outcomes from our study that better match the workforce skills identified in the previous study[11] as shown in **Figure 2**.

Participant Selection

For the recruitment of participants, we followed a random sampling method across various strata to ensure a diverse representation of chemistry doctoral programs throughout different regions of the United States. We compiled a comprehensive list of the 202 chemistry doctoral programs in the U.S., which were then categorized into five geographic regions: Northeast, Southwest, West, Midwest, and Southeast. We aimed to gather a sample of faculty that reflected a broad range of personal identities (including race and gender) and academic identities (such as area of interest, university affiliation, and academic rank). Following 19 interviews, we evaluated the distribution of participants concerning personal and academic identities to identify underrepresented groups in our sample, ensuring that diverse perspectives from all demographics were acknowledged and included.

Data Availability Statement

Per the IRB approval process, interview transcripts and resulting analyses are not made publicly available. However, supporting data have been included in the article's Supplementary Information.


Gender
Race_Ethnicity
Field
Rank
No. of Participants
0
5
10
15
20
23
19
2
1
20
13
4
3
3
2
9
7
6
5
5
5
4
3
1
17
14
13
1
Male
Female
Unknown
Non_binary
White
Asian
Hispanic/Latine
Mixed Race
Unknown
Black/African
Inorganic
Chemical Education
Materials/Polymer
Organic
Physical
Theoretical/Computational
Analytical
Biological/Biochemistry
Environmental
Associate
Assistant
Full
Emeritus
Demographics
Academic Background
Personal Background

	21st Century Skills Cluster (National Research Council, 2012)	Cui & Harshman Skills for Chemists (Cui and Harshman, 2020)	21st century skills needed for professional chemists	Codebook Skills
Cognitive Competencies	Cognitive processes and strategies	Planning and organizational skills Problem solving Critical thinking	Planning and organizational skills Problem solving Critical thinking	Planning or organizational skills Problem solving Critical or independent thinking
	Knowledge	Technical knowledge	Technical Knowledge	Technical Knowledge; Technical research skills
	Creativity	N/A	Creativity	Novel or significant research
Inter-Personal Competencies	Intellectual openness	N/A	N/A	N/A
	Work ethic/conscientiousness	Organizational awareness	Ethics & Organizational awareness	Career Preparation**; Ethics **
	Positive core self-evaluation	Personal value/attributes Personal growth/development	Personal value/attributes Personal growth/development	Affective outcomes** Mentorship (receiving); Evaluation and feedback**
Intra-Personal Competencies	Teamwork and collaboration	Teamwork/collaboration Networking skill	Teamwork/collaboration Networking skill	Networking/collaboration
	Leadership	Teaching skill Management skill Communication skill	Teaching skill Management skill Communication skill	Teaching skills Mentorship (learning how to mentor) Communication skills