Compressing Materials Development Timelines with AI - Greg Mulholland

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Executive Roundtable for Materials Growth

Hosted by: Growth Arc Advisors LLC and Kendall Justiniano, Managing Director

Contact Greg Mulholland (greg@citrine.io) for follow-up consultations for your organization.

Summary

Greg Mulholland came to materials AI the hard way. As a semiconductor engineer, he ran reactors growing gallium nitride — single tests costing hundreds of thousands of dollars — navigating largely on intuition and Excel. "It just felt like this is a crazy strategy." At Stanford he met a PhD materials scientist working in AI and machine learning. Greg's challenge was direct: do this with experimental data, not simulations, and you can change how the industry develops materials. Together they launched Citrine Informatics in 2014, first as a tech-enabled consulting firm, and now the leading AI platform for materials and chemicals development.

The central argument Greg made is that materials AI is not about breakthrough discovery. Materials companies run on know-how, process expertise, and operational excellence — the 85% margins that fund pharma's big-bet discovery model simply don't exist here. The job for AI is to make accumulated knowledge computable: data buried in old spreadsheets, heuristics in retiring experts' heads, relationships locked in decades of lab reports. "I think of AI as the very broad brain. I can't think about 50 things at the same time. AI can."

Why Materials Data is a Special Problem

AI has transformed supply chain, forecasting, and commercial operations at materials companies — but not R&D. The reason is structural. Experiments cost tens or hundreds of thousands of dollars, so data is sparse by design. And each data point can't be separated from the process that generated it: flatten a multi-step synthesis into a spreadsheet row and you lose what actually happened. "If you structure the data wrong, you structure the interesting things out of it."

Then there's the knowledge that never gets recorded at all. Retiring experts take decades of validated heuristics with them. Companies routinely re-run experiments they've already paid for because no one ever extracted the relationships from the original reports. A demographic gap — a thinner cohort of mid-career practitioners from a period when materials science was less popular — makes this more acute right now.

Greg identified five priorities currently driving AI adoption: reformulation away from PFAS and other regulated substances (now Citrine's largest area of business); faster time-to-market; cost optimization without sacrificing performance; expertise capture before a critical generation retires; and supply chain resilience — reformulating quickly around constrained inputs. The last two, he noted, weren't priorities Citrine anticipated when it launched in 2014. They emerged from the industry.

How Citrine's Platform Works

Citrine's platform has three integrated functions: understanding your data, incorporating what your scientists already know, and generating new formulations bounded by what can actually be manufactured. The input is materials properties and process data — typically spreadsheets that, as Greg put it, "look like they've been punched in the teeth," with gaps, missing provenance, and inconsistent structure. The system is built to work with that reality. The output is a ranked set of generative recommendations — hundreds of formulations or process conditions — with uncertainty quantification that distinguishes high-confidence predictions from more speculative ones. As Greg summarized: "Put in targets, get recipes."

The architecture uses graphical neural nets — a close relative of transformers — which handle long-range dependencies across multi-step processes: something done three steps ago can determine a property measured much later. The model operates within commercial constraints from the start: supply chain availability, process limits, banned ingredients, cost targets. "I'm not here to win a Nobel Prize. I'm here to create a commercially relevant product."

Expert knowledge enters through several channels: scientists input explicit relationships they already know, which the model projects into adjacent unexplored spaces; Omni Ingestre (an agentic tool) automatically extracts structured data from PDFs and datasheets; and Citrine's team works directly with client scientists to structure knowledge that isn't written down. The platform handles the blends-of-blends reality common in formulation science — unknown ratios, proprietary additives, incomplete ingredient data — rather than demanding clean inputs upfront.

Implementation: Starting Without Starting Over

When a company decides to move forward, Greg's first piece of advice is counterintuitive: don't start by reorganizing your data. Spending months cleaning and centralizing data before engaging AI consistently ends in expensive disappointment, because how you organize data and how you use it are tightly coupled — you can't know the right structure until you've used it. "If you have never done something before and you organize your entire garage around that thing, the likelihood you don't need to redo it is almost zero."

Citrine's approach: identify a high-value project, find the relevant data, and start. The model calibrates on the first cycle, improves on the second, and typically delivers strong results by the third. Most failures happen for one reason: teams refuse to iterate. They want proof before they test, which makes progress impossible. "It's like the kid who touches the stove. You can tell them a thousand times." Citrine's current success rate is 85–95% at the modeling level.

The people challenge is harder than the technology challenge. Scientists with 30 years of effective practice are skeptical; the change is real. The most effective approach: find enthusiastic teams first, get early wins, and let them evangelize internally. "The hard part is not the technology. It's helping people get their hearts and minds into a new approach."

Beyond the Lab: Commercial and Organizational Impact

The implications extend well beyond the lab. Application engineers and product developers — who typically spend weeks going back to R&D to determine whether a customer requirement is achievable — can instead arrive at candidate formulations before a customer call ends. "Hours versus weeks is the difference between getting the contract and not." Commercial teams shift from responding to requests to creating new conversations about what's possible.

Organizationally, the platform can couple expert knowledge across functions in ways that conversation alone can't scale. Greg's example: a crystallization expert and a processing expert can each load their knowledge and data into Citrine, then join them in a single model to optimize both at once. He called it the multi-physics analogy — the way CFD and FEA interconnect in simulation, extended to materials science. In large distributed organizations, this kind of systematic integration — and the permanent capture of the knowledge it produces — is a real structural advantage.

On data security: every client's data is fully siloed and never trains models for other customers; defense clients are covered under ITAR compliance. Looking ahead, natural language and agentic interfaces are already in internal testing — Greg described the demos as "a little bit mind blowing" — and represent the next step in lowering the barrier to entry for teams without deep data science resources.

About Greg Mulholland

Greg Mulholland is the co-founder and CEO of Citrine Informatics, the leading AI platform for materials and chemicals development. He founded Citrine in 2013 on the conviction that materials science was still discovering new materials the way Edison would have, and that AI could fundamentally change that. Under his leadership, Citrine has defined the field of materials informatics, earning recognition as a World Economic Forum Technology Pioneer, CB Insights AI 100 company, and World Materials Forum Startup of the Year.

He holds an MBA from Stanford, an MPhil in Materials Science from Cambridge, and a BS in Electrical and Computer Engineering from NC State, where he was a Park Scholar.

About Growth Arc Advisors LLC

After a 30 year career as an executive in the chemical industry, founder Kendall Justiniano started Growth Arc Advisors to help chemical business leaders implement the new thinking required for changing fundamentals. We're experienced industry operators who know the old playbooks, their gaps, and the new pages required.

The firm delivers customized engagements for Materials Executives in 3 key areas:

Commercial Effectiveness: increasing growth revenue through proven next-level commercial practices, including digital sales & marketing.

Strategy: helping clients navigate threats generated by sustainability, digital, and global demand shifts.

Innovation: accelerating return on innovation through focused investment.
