Tackling sustainable energy challenges with a Virtual Twin as a Service approach

A combination of advanced Geological, Material and Engineering modeling and simulations delivered by experienced technologists from Dassault Systèmes[2] has created a high value and cost effective paradigm in delivering efficient sustainable Energy solutions in record time

3DEXPERIENCE®

DASSAULT SYSTEMES

RESEARCH AND INNOVATION ARE KEYS TO UNLOCKING SUSTAINABILITY

The energy industry is accelerating research and innovation to meet sustainability goals. The following are some research areas that are being pursued:

- *Optimizing Extraction, Descaling*
- *Water Management*
- *Developing more Green Chemistry to meet Stricter Regulations*
- *New Formulations to reduce emissions*
- *Investigate permeability of CO_2 in various rock formations*
- *Improved CO_2 storage*

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DASSAULT SYSTEMES

SOLVING THE SUSTAINABLE ENERGY CHALLENGE WITH DASSAULT SYSTÈMES

In efforts to achieve profitable and sustainable energy operations, companies are often confronted with scientific challenges that require advanced software technology as well as experience in utilizing such technologies to achieve results rapidly. Dassault Systèmes has advanced geological, material science, data science modeling and simulation technologies that can solve numerous customer problems. Dassault Systèmes also realized that in addition to being able to solve problems there is also the factor of time-to-results. This often depended on having the right experienced scientific minds avail- able to apply the software. The need for rapid deployment and collaboration of the various Dassault Systèmes scientific technologies gave rise to the development of the Virtual Twin as a Service (VTaaS) framework described in this publication.

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KEY SOFTWARE TOOLS DEPLOYED AS PART OF THE VIRTUAL TWIN AS A SERVICE APPROACH

3DEXPERIENCE®

A COLLABORATIVE PLATFORM FOR LAUNCHING INTEGRATED APPLICATIONS AROUND A COMMON DATA AND SECURITY MODEL

- **Extraction Optimization- Pore-Scale Simulation= See customer Cases #1,#2**

Powered by DS's best-in-class Lattice Boltzmann physics, DigitalROCK® provides the first reliable, predictive technology for digital pore-scale simulation of relative permeability. The ability to accurately simulate two-phase flow, such as oil and water, through reservoir rock was co-developed and extensively validated with oil and gas industry leaders. Electric vehicle manufacturers and other major users of batteries can also benefit from using DigitalROCK to characterize the microstructure of the battery cell.

Available as a web-based application on the cloud, the streamlined DigitalROCK workflow goes from image to results easily and efficiently. Simulation enables unprecedented access to data for the engineers who need it. The user interface is easy and intuitive, and cloud delivery avoids infrastructure, hardware, and IT issues to minimize up-front expenses.

- **Advanced Materials- Modeling, Simulation and Data Driven Machine Learning for Next-Generation Materials- See Customer cases #3, #4**

Complete modeling and simulation environment designed to allow researchers in materials science and chemistry to predict and understand the relationships of a material's inherent chemistry with its properties and behavior.

Using Materials Studio, researchers in many industries are engineering better performing materials of all types, including catalysts, polymers, composites, metals, alloys, pharmaceuticals, batteries and more. It offers an "in silico first" approach, allowing researchers to optimize their materials' performance in a relatively low cost environment prior to physical testing.

Leveraging Dassault Systèmes Pipeline Pilot and its Collections, users author workflows in Pipeline Pilot, to deliver integrated, data-driven solutions, and potentially combine them with other Dassault Systèmes applications to augment out-of-the-box capabilities.

Our cutting-edge toolkit features a range of calculators, including COSMOtherm for predicting diverse properties, COSMOconf for conformer generation, COSMOperm for biomembrane permeability predictions, and COSMOquick for rapid COSMO-RS calculations. Dive into quantum chemical calculations with the TURBOMOLE1® component and seamlessly integrate COSMO databases for ef- ficient data access.

With readers, utilities, and a powerful COSMOplex extension, Dassault Systèmes provides a one-stop solution for advanced solvation chemistry. Elevate your research with precision and speed – the future of computational chemistry is here.

- **Sustainability- Advanced New Formulation Development for reduced CO2 emissions and in compliance with various regulations**

Unleashing Global Regulatory Compliance and Streamlined Lifecycle Management for Swift Market Success. Advanced formulation design provides for regulatory compliant, sustainable and cost effective formulations design. Organizations that manufacture formula-based products must ensure regulatory compliance globally and efficiently manage the complete lifecycle from idea to label. By facilitating the management of product complexity as well as the regulatory requirements for global formulations, Dassault Systèmes(DS)'s solution for Formulations Design and Management helps to improve productivity, manage costs and speed products to market.

Formulators get instantaneous regulatory guidance throughout formulation development and secure access to all current and historical product development data that significantly increases efficiency. Dassault Systèmes helps accelerate product innovation and product launches while successfully navigating complex regulatory requirements.

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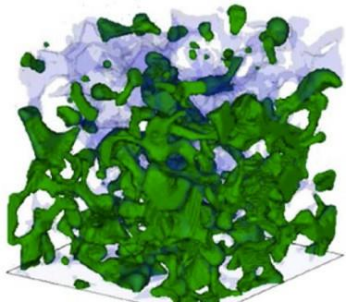
Customer #1

A large global energy company

GOAL



Mineral deposits formed from incompatibility between formation water and injected water impact fluid flow in reservoirs. Need to understand mechanism of deposit formation and design better inhibitors.

SOLUTION

Contract Research team used BIOVIA's chemistry-based solvers in Materials Studio for simulations of mineral phases and reactive transport to track the formation of scale deposits. Various scenarios were simulated, covering mineral types, phases, scale inhibitors, temperature and pressure conditions. In addition, output from these simulations were used as input into SIMULIA's DigitalROCK and to run multiphase Kr displacement simulations.

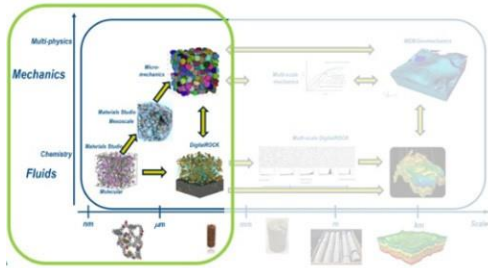
BENEFITS

- Actionable insights from virtual twin experiences not easy to obtain from experiments alone
- Justification for use of scale inhibitors in completion fluids

Customer #2

A large global energy company

GOAL



The objective is to eliminate challenges that impair infill wells from maximizing their true potential both for extraction and for CO_2 storage by optimizing fluid composition. need to rapidly screen injection locations, fluids and operational requirements to evaluate economic potential and accelerate final investment decision (FID)

SOLUTION

A combined Chemistry based simulations + Pore simulations approach was undertaken to address this need. Contract Research team used BIOVIA's chemistry-based solvers in Materials Studio for simulations of infill operations. Different fluid compositions at different temperatures and pressures were simulated. Using SIMULIA's DigitalROCK and database of properties from BIOVIA's chemistry-based results, reports were generated from permeability simulations.

BENEFITS

- Workflow developed and validated
- Save experimental time & cost by virtual design and optimization of fluid

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Customer #3

Largest Provider Of Products And Services To Energy Industry

GOAL

The need for a solution that implements efficient completion tools, ensuring secure CO_2 storage in challenging, erosive environments, and ultra-high geothermal conditions.

SOLUTION

Contract Research team performed simulations to study the impact of CO_2 on elastomer used as sealant and its effect on lifetime of the tool. Simulations of infiltration of CO_2 in different chemical environments, temperature and pressure conditions were also performed.

BENEFITS

- Prediction of sealant life for CO_2 injection operation in the presence of corrosive fluids.
- Better estimates of changes in mechanical properties to regulatory bodies for sealants near end of life.
- Use this information to differentiate Halliburton's CO_2 storage safety solution from competitors.

Customer #4

A Large Services Company to Energy Industry

GOAL

To better predict corrosion of metal assets under harsh conditions.

SOLUTION

Using client's data on corrosion of metal assets, Contract Research team was able to build predictive models using BIOVIA's Pipeline Pilot and Material Studio. The team was able to leverage chemistry-based descriptors to build machine learning models.

BENEFITS

- Decision-making dashboard allows engineers to rapidly determine what metal to be used for the purpose
- Better estimation of asset modification over a period of time

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OTHER VIRTUAL TWIN SUCCESSES

A FEW OTHER EXAMPLES WHERE VIRTUAL TWIN AS A SERVICE HAS SUCCESSFULLY MADE A DIFFERENCE TO OUR CUSTOMERS:

> Developing more Green Chemistry to meet Stricter Regulations

> Improved CO2 storage

> Refrigerant design to meet regulations

> New formulations for reduced emissions

> Scale formation and scale inhibitors

> Investigate permeability of Co2 in various rock formations

> Development of corrosion inhibitors

> Membrane design for separation

> Polymer and composite design

> Fuel Cell Membrane, Solid Oxide, and Electrode Design for Improving Efficiency while Reducing Cost

> Flow Assurance for Safer Transport

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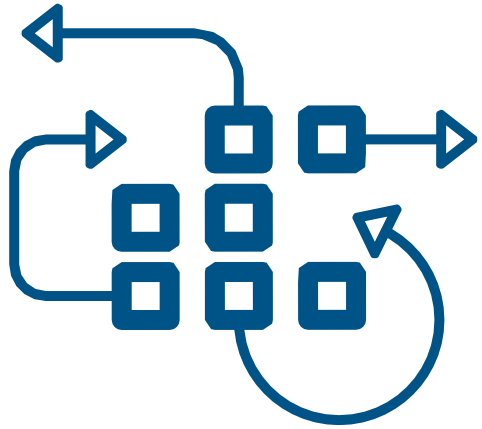
BREAKING YOUR SCIENTIFIC DEADLOCKS WITH VTaaS FRAMEWORK



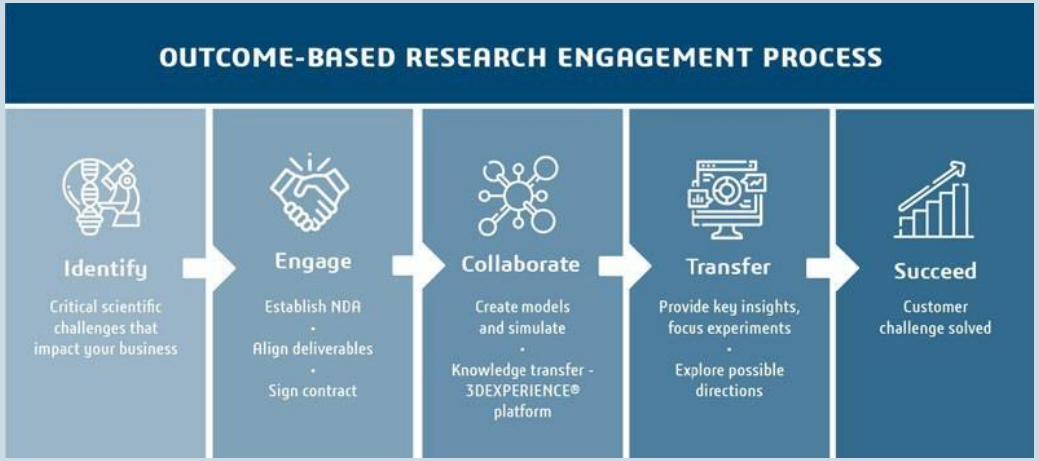
According to a McKinsey & Company, cutting emissions is not necessarily expensive if the Energy sector prioritizes the most cost-effective interventions. In fact, most of the emissions can be abated at an average cost of under US$50 per ton of carbon-dioxide equivalent (tCO2e). The pressure, hence, is for the research and development (R&D) organizations of energy companies to deliver more effective, on time and on budget innovations to drive the desired business outcomes.

Introducing Dassault Systèmes Contract Research Program

Dassault Systèmes Contract Research program via VTaaS framework is a contracted service dedicated to R&D organizations in large energy and materials companies. Offered as a flexible and collaborative scientific consulting and outcome-based research and development engagement, it uses 3D chemistry and physics based simulations and data science to accelerate innovation and optimization cycles, complemented by domain specific, multi-disciplinary experts to perform virtual "what/if" experiments on advanced software tools. This then frees the research team to focus on the most productive path to achieving its goals.

We bridge the capability gaps to help you:

- Innovate faster through virtual green chemical screening
- Design & optimize sustainable products and processes through V+R strategy
- Remediate failure through better understanding
- Obtain critical insights not possible from other means
- Shorten time-to-market of eco-friendly products



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ADVANTAGES

Contract Research program by **Dassault Systèmes** are performed under strict confidentiality. There are no surprises as price, deliverables and timeline are all agreed and fixed at the start. The engagement process leverages modeling, simulation, and machine learning to support accelerated innovation of eco-friendly product and solutions, through performance and process improvements that that save time, lower costs and help achieve sustainability goals

What you can expect

A jump-start to achieving valuable results in a short time frame

Relevant resources with expertise to help fill the gaps

A trusted partnership to extend your internal capabilities

A long-term working relationship

Typical ROI of more than 10 times

ADVANTAGES

UPSTREAM ENGAGEMENT

- Achieve higher yields through guidance from modeling toward the most successful and eco-friendly production path
- Lower investment risk for novel approaches through predictive modeling
- Reduce cost through virtual DoE
- Gain insights into production critical processes not obtainable from physical experiments or engineering scale models

DOWNSTREAM ENGAGEMENT

- Focus sustainable innovation toward the most successful path
- Understand at the nanoscale level for rational and green process improvement
- Exploit digital technologies to strengthen competitiveness
- Reduce cost and timelines and accelerate R&D to achieve sustain-ability goals

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SOLVE SCIENTIFIC CHALLENGES THROUGH OUR CONTRACT RESEARCH PROGRAM VIA VTaaS FRAMEWORK

Rational design outcome

In this approach, once validation is performed on the virtual models built, thousands of simulations are performed instead of many experiments. This virtual "design-of-experiments (DoE)" is much faster and "greener" since all the work involves simulation on high performance computers. A handful of the most promising virtual results are tested in the lab and only the best is taken forward. This way, a rational design outcome helps to cut down experimental time and cost and results in cutting the overall time by a third

EXAMPLE: CATALYST DESIGN OPTIMIZATION

This approach is what the VTaaS team employed for several catalyst design engagements. These range from catalyst used for po- lymerization and catalyst used for oxygen reduction reaction, to catalyst used in hydro-treating process (reducing Sulfur and Nitrogen emissions from fuels) and in many more cases

Critical insights outcome

We deploy deep-science chemistry-based simulation to better understand the material, chemical system and processes for oil and gas operations, as it is not always possible to conduct experiments in-situ due to the very harsh environments or extremely high temperature or pressure conditions at the site

EXAMPLE: SITUATIONS WHERE IT IS DIFFICULT OR EVEN IMPOSSIBLE TO GAUGE THE STATE OF A SYSTEM

This approach is applied by the VTaaS Contract Research team to over- come challenges ranging from enhanced oil recovery (EOR), materials safety issues, coatings design, process optimization, and much more, to gain critical insights into prohibitive environments via simulation

Innovation outcome

This approach leverages our multi-disciplinary expertise to bring knowledge from other scientific fields to overcome challenges in the energy sector. By combining the power of simulation with AI technology, we help research teams with "out-of-the-box" thinking, hypotheses generation, and virtual testing

EXAMPLE: PERFORMANCE-ENHANCED LUBRICANT

This approach is applied by the VTaaS team for performance enhanced lubricant, improving fuel cell membrane materials, liquid crys- tals with specific optical performance requirements, sensory perception improvement, sustainable replacements, indoor air quality improvements, efficient CO2 capture and storage, and much more

Root-cause analysis outcome

More often than one would expect, failure analysis becomes critical when a product has progressed to manufacturing or is already in the market. This approach combines deep-science chemistry-based simulation in conjunction with domain-specific feature engineered machine learning, to perform root cause analysis of a performance failure.

EXAMPLE: SOLVING ISSUES WITH SHELF-LIFE, MANUFACTURING, COAT- INGS FAILURE, ETC.

Root-cause analysis is applied to gain clarity into why a product is failing, and to discover ways to remediate, especially in situations where the fundamental reason for loss in performance cannot be verified by other means

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EXPECTED OUTCOMES FROM A PROVEN METHODOLOGY

Our methodology in combining multi-disciplinary expertise and software technology is tried and proven. With extensive use of artificial intelligence (AI) and data science, researchers can efficiently analyze scientific data, create machine learning models, generate virtual variants and screen rapidly. Our technique uniquely accounts for not just the experimental variables, but also the inherent chemistry of the system – to help different R&D teams deliver the desired outcomes for their business organizations

PROVEN AT THE UPSTREAM

Provided VTaaS Contract Research services to increase efficiency in oil recovery, minimize waste and reduce pro- duction costs, reduce environmental footprint, and meet new ecological standards, as well as strengthen competitiveness using digital technologies.

Successes

- Delivered solutions ranging from enhanced oil recovery to green hydrogen production. Examples include:
- Improving release agents for large scale EOR applications
- Identification of eco-friendly, sustainable replacements for flooding agents used for oil recovery
- Improving the viscosity modifier for pipeline transportation to facilitate operational oil production
- Gaining insights into why oil displacement depends on mineral type to improve recovering efficiency
- Development of a molecular switch for controlling water-oil emulsification and demulsification for heavy oil pipeline transport and water recovery
- Understanding key mechanisms of CO_2 storage in oil fields

PROVEN AT THE DOWNSTREAM

Provided engagement services to optimize performance of refining and purification processes, and to increase capacity through operational improvements, reduce waste and save costs. Also identified eco-friendly replacements that are not only sustainable but also aligned to ecological expectations.

Successes

- Delivered myriad chemical solutions to improve reaction efficiencies and overcome application challenges.
- Examples include:
- Rational designing of ionic liquids for carbon capture
- Virtual screening of porous materials for carbon capture
- Designing eco-friendly corrosion inhibitor for protecting steel pipeline
- Enabling selective removal of impurities and contaminants from hydrocarbon gas streams
- Reducing toxic waste by improving catalyst performance for hydrodesulfurization (HDS) and hydrodenitrification (HDN)
- Optimization of the GTL process

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WAYS TO ENGAGE WITH US

Through a flexible, milestone-based engagement process, you can contract a service from as basic as learning the best practices to apply our software to your needs (Jump-start Guidance offer), to as intensive as dedicating our resources to support your team for multiple years (Computational Scientist Resource offer).

The most popular type of engagement, however, is done project-by-project (Applied Research Project offer). Depending on your funding focus and the complexity of your challenges, we will set out clear deliverables, timelines and milestones, so that you attain your desired outcomes in planned phases that can range from three weeks to four months per phase.

By tapping on our deep scientific heritage and powerful technology expertise, you can enhance key knowledge and find the most innovative, sustainable and value-added solutions for the future.

THREE FLEXIBLE OFFERS TO LET YOU ENGAGE ON YOUR TERM

Computational Scientist Resource offer

- Dedicated off-site or on-site resource
- Managed by Contract Research p rogram Manager

Applied Research Project offer

- Innovative solution to specific scientific problems
- Deliverables mutually agreed before contract is signed
- Outcomes directly linked to actionable improvements, enhancements, and innovation

Jump-start Guidance offer

- Analysis of your scientific process to maximize value from Dassault Systèmes technology
- Guidance on applying licensed software to address specific problems

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Dassault Systèmes' is a **40 year old Global Software Company** and one of the largest software companies in the world with more than **22,000 passionate professionals** ready to collaborate and solve some of the biggest problems facing businesses today. **Dassault Systèmes**' global headquarters is located in Paris France, America's headquarters in Boston Massachusetts and Asia headquarters in Shanghai. We are Cloud first, platform based, PLM, **Science and Engineering Company**. **Covering 12 Industries** like Aerospace & Defense, Manufacturing and Energy and Materials.

Sustainability is at our core of who we are. **Dassault Systèmes** is currently ranked at #9 for most sustainable companies in the world. We are Industry Leaders in building **Virtual Twins**, using real world data to digitally replicate products, processes or assets and determine how they behave. Virtual twins enable reduced product life cycle times, improve manufacturing quality and control, and they drive more efficient use and recovery of resources across a product life cycle.

Dassault Systèmes By The Numbers

22,500+
Employees worldwide

€5.67 bn
Revenue in 2022

$44.6 bn
Market capitalization

197
Sites worldwide

#4
Ranking in the software sector by Dow Jones Sustainability Index

41%
R&D headcount

136
Countries with offices

> 20
Acquisitions in the past 5 years

More than 2/3
of the "brains" inside smartphones are designed using the 3DEXPERIENCE® platform

100%
of all planes, including solar-powered, are designed using the 3DEXPERIENCE® platform

Over 50%
of drugs and medical devices are designed using the 3DEXPERIENCE® platform

6 of the top 10
shoe companies in the world work with us

40%
of new clinical trials are supported by our solutions

40,000+
educational institutions work with 3DEXPERIENCE Edu

100%
of EV manufacturers are using our solutions

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