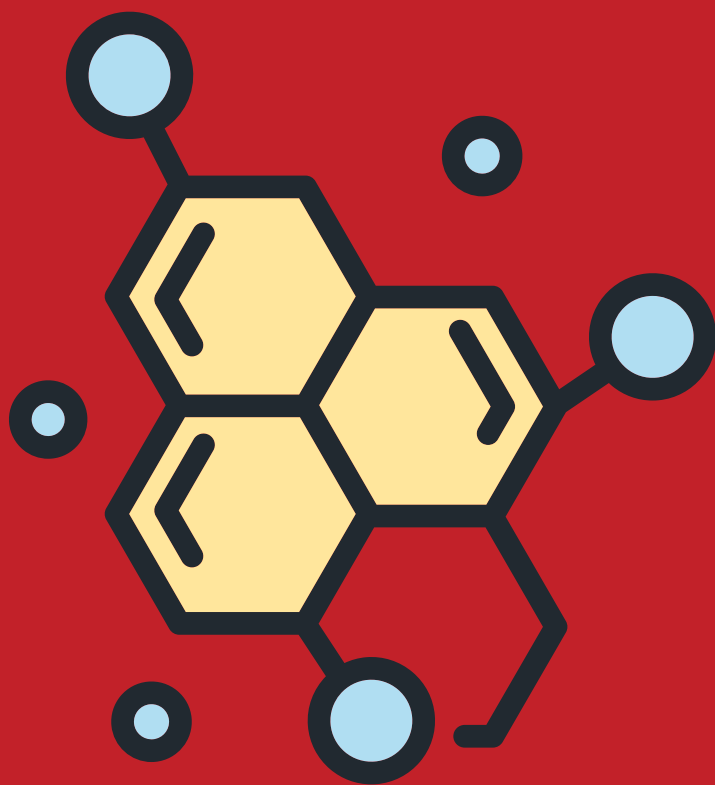




Driving Innovation in Chemical and Aftertreatment Systems Through Simulation

This eBook will cover the extensive capability of Gamma Technologies GT-xCHEM for chemical and exhaust aftertreatment systems modeling.

eBook

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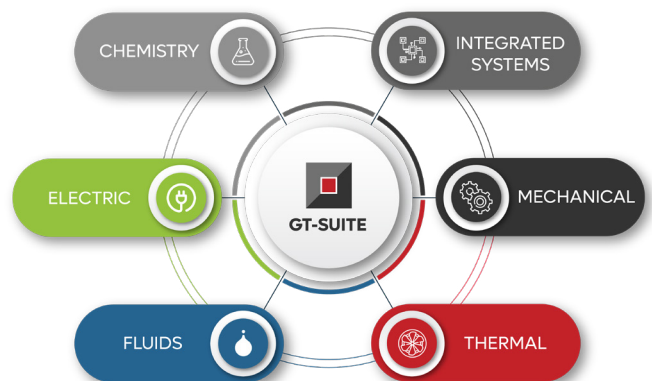
TACKLING EMISSION CHALLENGES WITH CAE



The urgency to combat pollution and climate change has never been more pressing. According to the World Health Organization (WHO), 99% of the global population breathes air that exceeds WHO guideline limits, as reported in 2022. Automotive and industrial activities are a major driver of rising greenhouse gas emissions, and as the impacts of pollution intensify, innovative engineering solutions are crucial to mitigate these environmental challenges.

Computer-Aided Engineering (CAE) tools enhance the precision and speed of the design process, allowing for the simulation of complex chemical reactions and processes, ensuring optimal performance before physical implementation. CAE tools such as GT-xCHEM and GT-SUITE, play a pivotal role in addressing environmental challenges. These powerful platforms provide advanced capabilities for aftertreatment and chemical systems modeling, enabling engineers to design highly efficient systems that reduce harmful emissions.

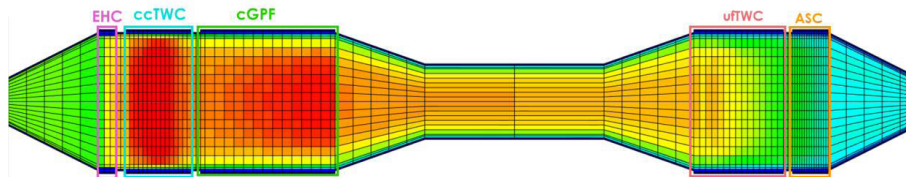
In addition to these capabilities, GT-SUITE supports the development of net-zero carbon technologies, such as fuel reformers, fuel synthesis, and carbon capture. CAE enables engineers to create sustainable, low-carbon energy solutions, advancing the global push for cleaner energy systems. This eBook explores how GT-xCHEM and GT-SUITE are helping engineers design solutions that not only meet stringent environmental regulations but also drive the transition to a more sustainable, net-zero carbon future.



Multi-physics Capabilities with GT-SUITE

ROLE OF SIMULATION IN MODELING AFTER-TREATMENT SYSTEMS FOR SUSTAINABILITY

Modeling exhaust aftertreatment systems to address diverse emission control challenges with precision and efficiency is a complex task, requiring engineers to develop systems that meet stringent emission standards while optimizing performance and reliability. Achieving this requires comprehensive tools that can handle the intricate dynamics of chemical reactions and system behaviors within aftertreatment systems.

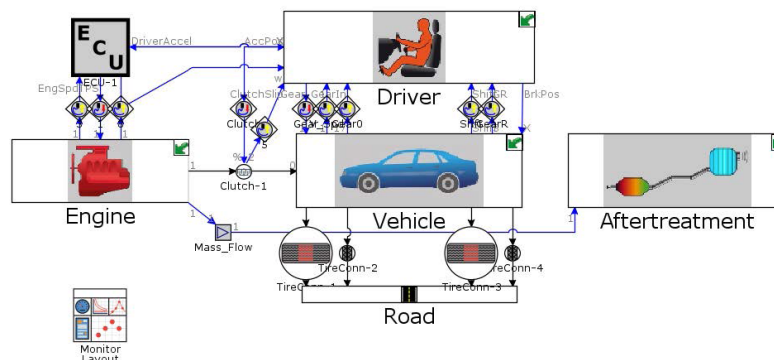


Exhaust Aftertreatment Model in GT-xCHEM

Gamma Technologies offers GT-xCHEM, a comprehensive platform for modeling and simulating exhaust aftertreatment systems. GT-xCHEM's advanced simulation capabilities are crucial for accurately modeling various aftertreatment systems, including electric heating catalysts, three-way catalysts, and advanced particulate filtration. The tool excels in simulating intricate chemical reactions, thermal behavior, and flow non-uniformities. A critical feature is its flexible reaction mechanism templates, which allow users to define custom mechanisms or use well-calibrated examples as starting points. Integration with GT-SUITE enhances its utility by combining subsystem models into unified system-level simulations, facilitating a holistic evaluation of system interactions and trade-offs such as:

- NOx vs. PM emissions
- Thermal boundary conditions for engine control
- Control strategy optimization

With features like faster-than-real-time quasi-steady flow solvers, intuitive interfaces, and advanced post-processing, GT-xCHEM provides unmatched ease and precision in aftertreatment solutions. Engineers can utilize these capabilities to optimize emission control strategies and evaluate the impact of various system interactions effectively.



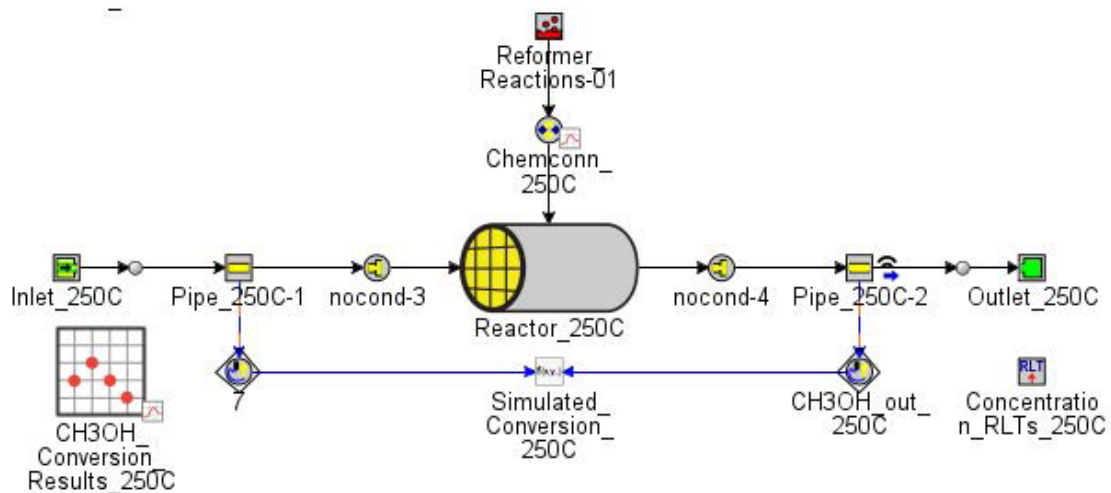
Engine Vehicle Aftertreatment System Model in GT-SUITE

ENHANCING CHEMICAL SYSTEM DEVELOPMENT THROUGH SIMULATION

Engineers are challenged to find versatile platforms for chemical systems modeling across industries, capable of simulating complex reactions accurately. Reliable and efficient solutions are essential for tackling intricate chemical engineering challenges with precision.

Gamma Technologies provides a platform for chemical system modeling, supporting various processes, including:

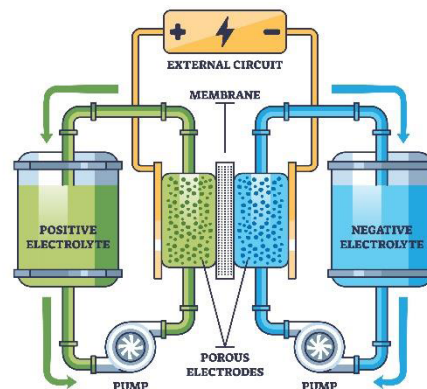
- **Fuel Reformers and Reaction Modeling:** GT-xCHEM models reformers for hydrocarbon fuels like methane, ethanol, methanol, along with ammonia cracking processes. It supports critical reactions like the water-gas-shift and reverse water-gas-shift reactions. Engineers can model reformers as standalone systems or integrate them into broader system-level simulations.



Methanol Reformer Model in GT-SUITE

- **Advanced Distillation Column Modeling:** The 2025 version of GT-SUITE introduces distillation column modeling, enabling detailed simulations and optimization for chemical processing systems.
- **Electrolytic Fluid Flow Systems:** Enhanced modeling capabilities predict electrochemical corrosion, wall degradation due to corrosion, electrical potential distribution along pipe walls, etc. New templates, such as reactive ducts, electrolyte solutions, solvents, and more, facilitate these simulations. Applications include carbon capture, electrolyzers, redox flow batteries, and marine wet scrubbers.

- **Flow Battery Simulations:** Flow batteries, a large-scale electrochemical energy storage system, are modeled for renewable energy storage. These batteries, with their long lifespan and suitability for stationary applications, store energy in electrolytes pumped across anodes and cathodes to generate electricity.



Flow Battery Model

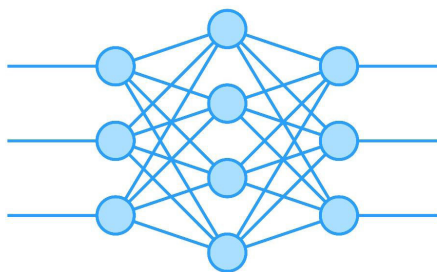
Engineers can leverage GT-xCHEM to design and optimize innovative chemical systems across industries. For example, fuel reformers enhance the production of hydrogen from renewable feedstocks, while distillation columns optimize chemical separation processes. Electrolytic fluid flow modeling aids in carbon capture and corrosion prediction, and flow battery simulations address renewable energy storage challenges. By offering precise and scalable solutions, GT-xCHEM helps drive innovation in chemical systems engineering.



Flow Battery Installation for Large-Scale,
Long-Duration Energy Storage

MACHINE LEARNING FOR CHEMICAL SYSTEM MODELING AND OPTIMIZATION

With the need for faster simulations and optimized designs growing, traditional methods are no longer sufficient. Machine learning integration is crucial to accelerate analysis and refine designs. A tool with inbuilt machine learning capabilities is essential for streamlining workflows and improving efficiency.



Visual Representation of a Multi-Layer Neural Network

The in-built machine learning assistant of GT-SUITE meets the growing demand by enabling:

- **Faster Simulations:** The tool facilitates rapid-running plant models for multiphysics simulations, hardware-in-the-loop simulations, and design optimization.
- **Resource Efficiency:** Lightweight mathematical models can be deployed on microcontrollers, ECUs, or low-power devices, ensuring performance even in constrained environments.
- **Metamodeling Techniques:** GT-xCHEM with GT-SUITE supports dynamic and static metamodels, using methods like polynomial regression, Gaussian interpolation, and neural networks. Neural networks, including multi-layer perceptrons and non-linear autoregressive exogenous models (NARX), effectively capture intricate system dynamics.
- **Enhanced Decision-Making:** As a design tool, GT-xCHEM with GT-SUITE helps engineers understand complex relationships between inputs and outputs, leading to more informed and accurate decisions.

Machine learning finds practical applications in:

- **Dynamic Reactor Modeling:** By combining dynamic and static neural networks, GT-xCHEM simulates the behavior of aftertreatment reactors with high accuracy.
- **CFD-Driven Predictions:** Models trained on Computational Fluid Dynamic (CFD) data predict concentration distributions at the SCR inlet, improving precision in system performance evaluations.
- **Stoichiometric Ratio Analysis:** Case studies demonstrate the use of neural networks to determine stoichiometric ratios with exceptional reliability, showcasing their application in real-world scenarios.

These capabilities empower engineers to accelerate design cycles, reduce development costs, and bring innovative solutions to market more effectively. GT-xCHEM with GT-SUITE ensures that advanced chemical kinetics modeling is not only precise but also practical for modern engineering challenges.

LEVERAGING SIMULATION FOR FUEL REFORMING, SYNTHESIS, AND CARBON CAPTURE FOR NET-ZERO GOALS

Engineers face the challenge of driving sustainable engineering to achieve a net-zero carbon future. Developing advanced technologies for alternative fuel production, carbon capture, and energy efficiency requires a versatile and reliable solution. The need for a platform that supports these efforts and empowers engineers to meet carbon-neutral objectives is crucial for making impactful progress.



Carbon Capture and Storage Concept

GT-SUITE provides robust tools for:

- **Alternative Fuels and Fuel Reformers:** Hydrogen and ammonia are pivotal to the next generation of alternative fuels. GT-xCHEM enables precise modeling of chemical reactions for renewable feedstocks like methane, methanol, and ethanol. It supports standalone or integrated modeling of fuel reformers, including reactors like Haber-Bosch and Auto-Thermal Haber-Bosch for ammonia synthesis
- **Green Methanol Production and Applications:** GT-SUITE facilitates green methanol production simulations, scaling from lab setups to industrial reactors by incorporating subsystems like wind turbines, solar panels, and carbon capture units

Methanol serves as a transportable fuel with varied applications:

- **Internal Combustion Engines:** Methanol powers flex-fuel vehicles, including hybrids
- **Fuel Cells:** Used directly in DMFC or reformed into hydrogen for RMFC
- **Blending Component:** Blended with gasoline or diesel, such as in M85 (85% methanol)

Carbon capture technologies; GT-SUITE supports cutting-edge simulation of:

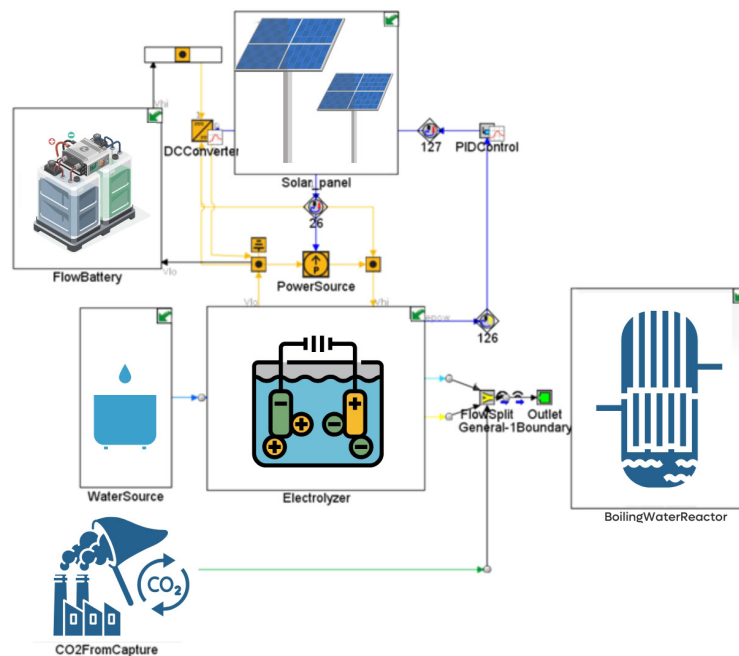
- **Physical and chemical adsorption/absorption**
- **Direct Air Capture (DAC)**

For mobile and marine applications, GT-SUITE simulates CO₂ capture, covering cooling, liquefying, drying, and storage. In the near future, GT-SUITE will also include capabilities for simulating cryogenic processes and membrane-based separation.

The practical applications of GT-SUITE in achieving a net-zero carbon future include:

- **Fuel Reformers and Synthetic Fuels:** Efficient hydrogen and ammonia production systems, coupled with methanol-powered engines and green methanol production, showcase the versatility of GT-SUITE in promoting alternative fuels
- **Carbon Capture Solutions:** Simulations of adsorption/desorption processes enable engineers to design CO₂ storage solutions for industries and vehicles. Mobile carbon capture technologies for cars, trucks, and ships highlight its adaptability, offering insights into power consumption, mass penalties, and efficiency trade-offs

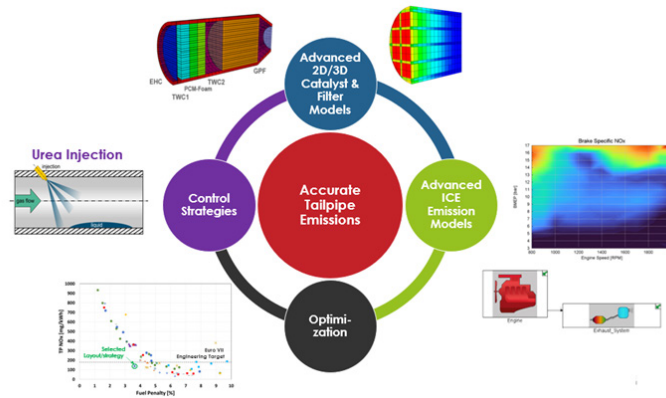
GT-SUITE's comprehensive simulation capabilities guide engineers in innovating and optimizing sustainable systems, paving the way for a cleaner, carbon-neutral future.



System Level Model for e-Methanol Production

ADVANCED SIMULATION CAPABILITIES FOR AFTERTREATMENT MODELING

Thermal management is a crucial aspect of maintaining the performance of aftertreatment systems and ensuring compliance with emission standards. The integration of advanced thermal management techniques and sophisticated modeling capabilities plays a vital role in optimizing these systems.

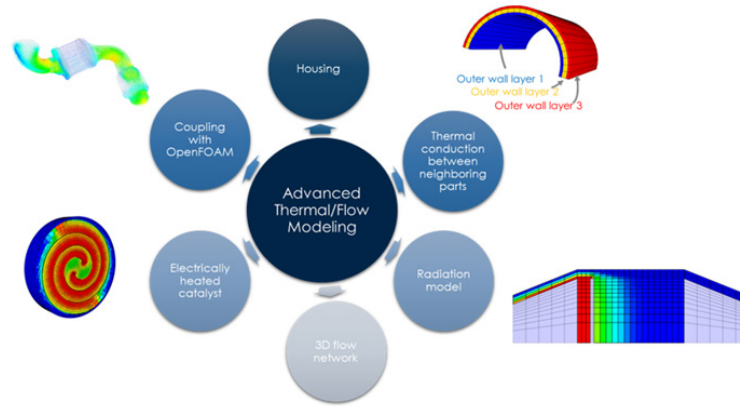


GT Emission Solutions

Aftertreatment systems, involves technologies like electrically heated catalysts, burners, and secondary air pumps, which are especially beneficial during cold starts. The design and optimization of system components and aftertreatment boxes help maintain ideal temperatures by minimizing thermal losses. Additionally, phase change materials (PCMs) are instrumental in preventing system cool-down during engine shutdowns, a feature particularly important for hybrid vehicles.

GT-xCHEM excels in modeling the complete aftertreatment system on a unified platform, providing capabilities such as:

- **2D/3D Catalyst and Filter Modeling:** Allows detailed simulation of catalysts and filters
- **Integration with Engine Models:** Enables coupling with detailed engine simulations for holistic system analysis
- **Control Logic and Optimization:** Facilitates the development of sophisticated control strategies to accurately predict tailpipe emissions
- **Comprehensive Component Modeling:** GT-xCHEM can model ducts, monoliths, filters, sensors, injectors, electrically heated catalysts (EHCs), and assemblies, ensuring a thorough representation of the aftertreatment system
- **Coupling with CFD Analysis:** The models can be linked with CFD simulations performed in OpenFOAM to include boundary conditions, pressure drop, energy balance, and detailed chemical reactions
- **Thermal Analysis for System Optimization:** GT-xCHEM incorporates comprehensive thermal analysis to maintain optimal temperatures throughout the system. This includes evaluating thermal conduction, radiation, and the dynamic thermal behavior of components under varying operational conditions. The insights from these analyses help in minimizing heat loss, optimizing thermal shielding, and ensuring effective use of phase change materials (PCMs) for enhanced thermal efficiency



Advanced Thermal/Flow Modeling

By providing these advanced capabilities, GT-xCHEM empowers engineers to design aftertreatment systems that meet emission standards while optimizing performance, efficiency, and reliability.

Conclusion:

This eBook delves into the advanced simulation and machine learning capabilities of GT-xCHEM and GT-SUITE in optimizing chemical and aftertreatment systems. These tools facilitate precise modeling of chemical reactions, emissions, fuel efficiency, thermal management and more, while supporting the development of alternative fuels and carbon capture technologies. By integrating machine learning for faster simulations, they empower engineers to meet stringent environmental standards and drive innovation towards sustainability.

IF YOU'RE INTERESTED TO LEARN MORE

Want to accelerate your simulation process and cut down development time? Our advanced multi-physics tools, incorporating thermal, flow, electrical, mechanical and control systems, optimize the entire simulation workflow. By integrating machine learning and enabling seamless system integration, we help you reduce time-to-market and improve performance.

Get in touch to learn how our solutions can streamline your engineering projects.

ACCESS
HERE

GT-xCHEM

GT-xCHEM is an advanced simulation tool within GT-SUITE, designed for modeling complex chemical reactions in exhaust aftertreatment and chemical systems. It excels in simulating intricate interactions, offering flexible reaction mechanism templates, thermal management, and system integration.

ACCESS
HERE

GT-SUITE

GT-SUITE is the industry-leading simulation tool with capabilities and libraries aimed at a wide variety of applications and industries. It offers engineers functionalities ranging from fast concept design to detailed system or sub-system/component analyses, design optimization, and root cause investigation.

ACCESS
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TRAININGS & SEMINARS

GT is committed to providing the best possible training and customer support to all users of GT-SUITE. This includes making sure that GT users have the information they need to solve their simulation challenges. To help users get the most out of GT-SUITE, we offer a series of videos to help users with common challenges.



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