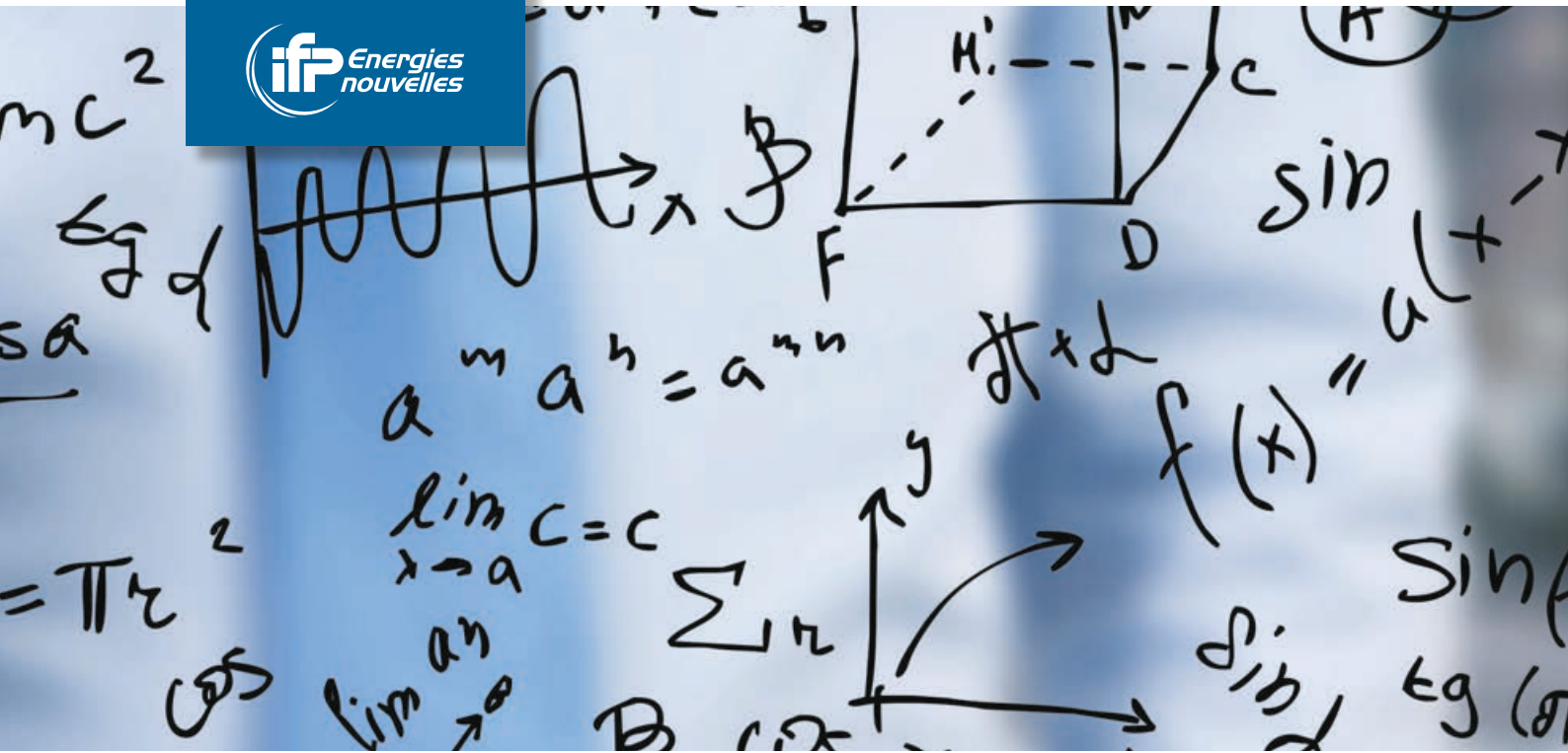
FUNDAMENTAL RESEARCH



Serving innovation

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IFP Energies nouvelles

IFPEN is a French public research and training player. It has an international scope, covering the fields of energy, transport and the environment. From research to industry, technological innovation is central to all its activities.

As part of the public interest mission with which it has been tasked by the public authorities, IFPEN focuses on:

- providing solutions to take up the challenges facing society in terms of energy and the climate, promoting the transition towards sustainable mobility and the emergence of a more diversified energy mix;
- creating wealth and jobs by supporting the competitiveness of related industrial sectors.

IFPEN's programs are hinged around three strategic priorities:

- Sustainable Mobility: develop effective, environmentally-friendly solutions for the transport sector;
- New Energies: produce fuels, chemical intermediates and energy from renewable sources;
- Responsible Oil and Gas: propose technologies that meet the demand for energy and chemical products while improving energy efficiency and reducing the environmental impact.

An integral part of IFPEN, its graduate engineering school – IFP School – prepares future generations to take up the challenges of the energy transition.

Ambitious fundamental research…

IFPEN's fundamental research is designed to promote and accelerate the emergence of technological innovations.

Structured

The challenges associated with the energy transition give rise to a broad range of open scientific questions. To address these questions in a coherent and transparent manner, IFPEN's fundamental research activities have been structured around nine scientific challenges. By focusing the research effort, this organization is designed to accelerate the acquisition of knowledge and feed the innovation process.

IFPEN's nine cross-functional scientific challenges

Experimentation, data acquisition, understanding

1. Material and fluid characterization
2. Reaction mechanisms
3. Containment effect
4. Massive data flows

Physical models and descriptors for simulation

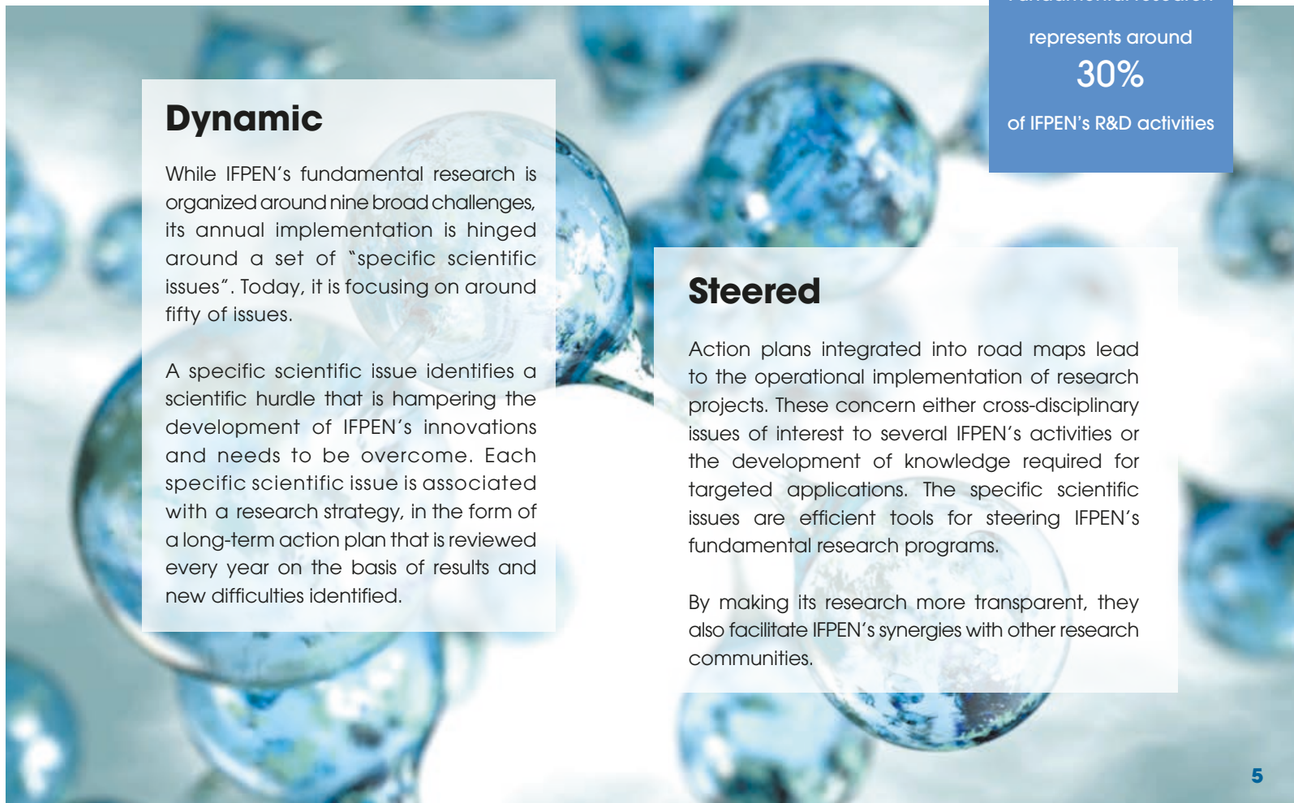
5. Descriptors
6. Modeling of coupled phenomena

System simulation, optimization or commands

7. Command and optimization
8. Code performance

Economic and environmental challenges of the energy transition

9. Economic and environmental assessments



Fundamental research represents around **30%** of IFPEN's R&D activities

Dynamic

While IFPEN's fundamental research is organized around nine broad challenges, its annual implementation is hinged around a set of "specific scientific issues". Today, it is focusing on around fifty of issues.

A specific scientific issue identifies a scientific hurdle that is hampering the development of IFPEN's innovations and needs to be overcome. Each specific scientific issue is associated with a research strategy, in the form of a long-term action plan that is reviewed every year on the basis of results and new difficulties identified.

Steered

Action plans integrated into road maps lead to the operational implementation of research projects. These concern either cross-disciplinary issues of interest to several IFPEN's activities or the development of knowledge required for targeted applications. The specific scientific issues are efficient tools for steering IFPEN's fundamental research programs.

By making its research more transparent, they also facilitate IFPEN's synergies with other research communities.

... implemented and **expressed** in a variety of forms

Working with leading partners

In order to develop the solutions and industrial sectors of the energy transition, IFPEN has been involved in the French Research and Innovation System (SFRI) since its creation by the public authorities and participates in numerous collaborative projects. IFPEN also brings its expertise and skills to major projects on a European level (ERA).

- ANR*-funded projects: 3 new projects selected for funding in 2019
- More than 300 collaborations with French and international academic partners
- H2020-funded projects: 29 projects selected for funding since 2014
- 5 visiting scientists and 14 visiting PhD students hosted since 2017

*French National Research Agency

Constant rejuvenation thanks to young researchers

Research-based training at IFPEN offers students and young researchers the chance to join one of its R&D divisions and work for a fixed period within a stimulating research environment, with access to first-class laboratory infrastructures and computing facilities.

Internship program
Opportunities for French and international students: internships typically lasting 4 to 6 months.

Doctoral studies program (PhD)
More than 40 new doctoral research projects started every year in cooperation with French and international universities: all PhD students are part of IFPEN's Doctoral College and have access to dedicated seminars and training sessions.

Postdoc program
Postdoc positions are available for PhD holders who have obtained their degree within the past three years.

To apply for these opportunities: training@ifpen.fr
More information at: www.ifpenergiesnouvelles.com/training-and-careers/training-through-research

Networking and outreach

IFPEN maintains its high level of excellence by promoting exchanges between its researchers and the scientific community via international scientific events, relating to emerging or recurrent topics and designed to:

- offer a dynamic and attractive forum for research teams,
- forge contacts for future collaborations.

A new event format was launched in 2018; the Scienc'Innov Workshops are more particularly dedicated to the specific challenges of the fundamental research program.

In 2019, scientific events organized by IFPEN included:

Microfluidics 2019: from laboratory tools to process development (IFPEN scientific event)

e³CAV: Connected and Automated Vehicles for Energy Efficiency and the Environment (IFPEN Scienc'Innov workshop)

MASCOT-NUM 2019: annual conference of the French National Center for Scientific Research (CNRS) "Mascot-Num" research group, focused on data assimilation, uncertainty quantification, statistics and numerical analysis

3rd European Workshop on the Bioeconomy: co-organization with INRAE

Events planned for 2020 include:

Scale4Mat: innovative materials: which scale-up methodology? (IFPEN Scienc'Innov workshop)

Corrosion in Low Carbon Energies (IFPEN Scienc'Innov workshop)

ESAT 2020: 31st European Symposium on Applied Thermodynamics, co-organized with Mines Paris Tech engineering school

Coupling CFD and thermodynamics: thematic workshop of the SFGP (Société française de génie des procédés – French Process Engineering Society)

The dissemination of its scientific research is another way for IFPEN to make its R&D results accessible to all and to allow the scientific community to harness them.

Publications in scientific peer-reviewed journals: around 200 per year

OGST: open access journal for which IFPEN leads the editorial committee, covering all disciplines and fields relevant to energy production, conversion, storage and use

Science@ifpen: a quarterly newsletter presenting scientific and technical results obtained by IFPEN's research teams through internal and collaborative activities

News feed: short news items, published on the IFPEN website and relayed on Twitter

Follow us: @IFPENinnovation

Cutting-edge scientific skills
and resources...

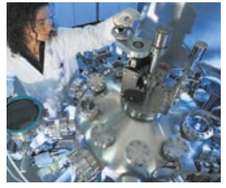
IFPEN's employees form a unique body of recognized scientific specialists from around the world and an unparalleled network of expertise in a broad variety of fields.

Geosciences

Geology - Sedimentology
Geochemistry
Geostatistics - Geological modeling
Geomechanics
Petrophysics and transfers in porous media

Chemical sciences

Catalysis and reaction kinetics
Organic and mineral synthesis
Separation and adsorption techniques
Theoretical chemistry



Analysis and characterization

Chemical analysis
Structural analysis and imaging
Mechanical testing
Microfluidics
High-throughput experimentation (HTE)

Physical sciences

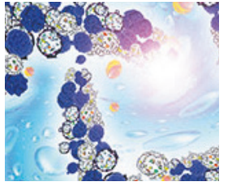
Transfer and transport physics
Rheology and behavior of materials
Thermodynamics/Molecular modeling

1,120
researchers

11,800
active patents

2019: 185
basic patents including 94 in the field of new energies

Around 170
publications per year in the Science Citation Index

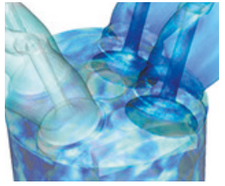


Physical chemistry

Complex fluids, colloids and condensed matter
Surface, interface and materials science
Electrochemistry and corrosion

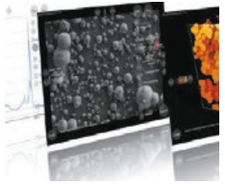
Biosciences and biotechnologies

Microbiology
Genomics
Biocatalysis
Fermentation



Engineering sciences

Solid mechanics
Fluid mechanics
Chemical and process engineering
Combustion and engine technologies
Electrical and electronic engineering
Automation and control systems
Systems modeling and simulation



Mathematics and IT

Numerical methods and optimization
Signal processing - Data science
Meshing and visualization
Software design
Real-time systems
High performance computing
Bioinformatics

Economics

Microeconomics and econometrics
Macroeconomics
Economic modeling
Forecasting and scenario modeling
Technical and economic evaluation
Environmental impact evaluation & LCA

... spread over more than **thirty departments**

2018-2019

scientific highlights

Plug im!: a deep learning image processing platform

Designed by IFPEN, plug im! is a modular platform providing non-expert users with access to 2D and 3D signal and image processing. User-friendly, it also incorporates modules provided by industrial and academic partners. In particular, the platform enables automatic batch processing of multiple data without the need for a single line of code. Available on an open access basis, it recently acquired a deep learning method which has proved effective when employed for the detection of defects in different types of alumina catalyst supports. On the back of this success, IFPEN has launched further projects aimed at transposing this approach, which opens up a new avenue in the field of data science.

CARMEN: the new joint research laboratory with the CNRS

For nearly 40 years, IFPEN and the CNRS have been working together on doctoral and post-doctoral research projects and within the context of joint research groups. In 2018, the renewal of the framework agreement defining their collaboration led to the creation of the CARMEN (*CARactérisation des Matériaux pour les Énergies Nouvelles*) research laboratory, which also involves Claude Bernard Lyon 1 University, ENS Lyon, Sorbonne University, and Strasbourg University. The purpose of this new entity is to reinforce knowledge on molecular and/or colloidal transport in porous substrates and develop new methodologies for the detailed analysis of these materials in order to support the development of innovations for the energy transition.

Launch of the ROAD4CAT chair in the field of catalysis

The ROAD4CAT (RatiOnAl Design for CATalysis, IDEXLYON's first industrial chair) agreement was signed in June 2018 with Lyon University. The chair, bringing together IFPEN and the chemistry laboratory at ENS Lyon, proposes a fundamental research approach based on computational chemistry applied to the rational design of heterogeneous catalysts. It hosts research projects aimed, on the one hand at identifying new concepts governing the genesis of heterogeneous catalysts and, on the other hand, at exploring new approaches in the fields of biomass conversion and photocatalysis. The chair holder delivers courses (64 hours) at a Master level in the thematic fields of the chair.

The success of the Oxygen JIP leads to the Fugacity JIP

Alongside the Institut de la Corrosion de Saint-Étienne (French Corrosion Institute in Saint-Étienne), IFPEN led the Oxygen Joint Industry Project (JIP) aimed at addressing the issue of the reliability of choices of materials for oil and gas transport. The program successfully evaluated the impact of oxygen traces on steel corrosion in the presence of H_2S while making it possible to anticipate steel corrosion and fracture risks in an EOR context and in some new energy technology fields, such as geothermal energy and biogas. Following on from this work, the Fugacity JIP is focused on the effect of high pressures (transient effects) on the penetration of hydrogen resulting from the steel corrosion process in the presence of CO_2 and H_2S.

Launch of the new EleTher JIP on thermodynamic modeling

A survey of the "Thermodynamics and Transport Properties" working party of the European Federation of Chemical Engineering (EFCE) had identified some major gaps in the understanding of systems containing ionic species. In the light of this, IFPEN, together with some industrial partners, has launched the EleTher JIP. Dedicated to the thermodynamic modeling of electrolyte containing systems, it is aimed at proposing a method for analyzing existing data with a view to developing extrapolation methodologies and establishing a procedure to determine thermodynamic model parameters. In particular, its results will lead to a better understanding of specific phenomena for the purpose of products and processes development in various fields: biomass transformation, batteries design, CO_2 capture and storage, prevention against corrosion of equipment and structures.

2018-2019

scientific highlights

Mascot-Num: a long-standing research partner in the field of stochastic methods for the analysis of numerical codes

The aim of the Mascot-Num research group is to promote and improve the research in the scientific field of data assimilation, uncertainty quantification, statistical techniques for machine learning and the analysis of computer experiments. Its 14th annual conference was held in March 2019 at IFPEN, whose fundamental research is particularly concerned by these areas. For instance, IFPEN developments in intersection with the research group are: model calibration, reliability, metamodeling, dimension reduction and optimization. The event was an opportunity for researchers to present progress made in these areas and discuss the latest developments with specialists in the corresponding fields.

ANCRE: IFPEN leads three exploratory projects for energy

Three projects initiated by IFPEN, a founding member of the French National Alliance for Energy Research Coordination (ANCRE), were selected within the context of the call for projects on the theme of "basic sciences for energy". One of these, Transmet, conducted in partnership with Paris-Saclay University, is aimed at developing a methodology for building a model used to predict ion and water transport properties in the saline aqueous phase. The other two, Erbag and the RME network, conducted in partnership with Lorraine University, respectively concern the characterization and understanding of phenomena associated with bacteria flow and retention in porous media and the development of magnetic resonance methods in the energy field.

The IPPAD project closes

The IPPAD fundamental research project, conducted within the context of the ITN-MSCA Horizon 2020 program, ended after four years of research work. It focused on the behavior in ultra-high-pressure condition a fuel in the presence of additives, as well as the impact of phase change (liquid/gas/solid) on soot emissions in Diesel engines. Central to this program were two IFPEN theses: the first developed a model for the injection of fuel in sub-critical and super-critical conditions using an innovative thermodynamic approach, while the second was dedicated to the mechanisms of soot formation and oxidation via a multiscale approach combining macroscopic kinetic simulations and atomistic calculations. These doctoral studies led to publications in major scientific journals.

More efficient photocatalysts for capturing solar radiation

Researchers from the CNRS, the University of Bordeaux and IFPEN have developed new catalytic materials capable of effectively capturing and converting the photons from solar radiation, an approach with significant potential when it comes to addressing energy challenges. The originality of the developed solution lies in a tailor-made volume configuration of these photo-active materials rather than the standard two-dimensional form (thin layer). This makes it possible to significantly improve the CO_2 conversion performance of the photo-driven systems and to reduce their footprint. In recognition of this research, the results of which have a significant impact on "solar fuel" production systems in the field of photo-active systems, Sophie Bernadet received a thesis innovation award from the French Chemistry Society's Energy Inter-division.

Did you **know?**

IFPEN is committed to implementing an ethical and rigorous scientific approach when conducting its research activities. In 2018, it established a scientific integrity policy, signing up to the "National Ethics Charter of the Research Professions" and appointing a "scientific integrity" officer, responsible for training personnel and promoting good practices relating to the conduct of research and the publication of results.

IFPENS's scientific publications have been available for consultation on an open-access basis on the HAL-IFPEN platform since 2012.

IFPEN research: **award winners** in 2018 and 2019

Sophie Bernadet, former IFPEN PhD student, 2019 thesis innovation prize awarded by the French Chemistry Society's Energy Inter-division

Céline Chizallet, 2018 young researcher prize awarded by the Catalysis Division of the Société chimique de France (French Chemistry Society)

Éric Deville, 2019 prize awarded by the French Isotope Society (SFIS) for the best article written by a French-speaking researcher

Alexandre Lettéron, former IFPEN PhD student, 2018 thesis prize awarded by the Association des géologues du Sud-Est (South-East Geologists Association)

Xavier Mangenot, former IFPEN PhD student, 2018 Van Straelen thesis prize, awarded by the French Geological Society

Benoît Noetinger, the Rheims Foundation's 2019 Adrien Constantin de Magny Prize

Céline Pagis, recipient of the 2018 L'Oréal-Unesco "For Women in Science" fellowship, 2019 Denise Barthomeuf Prize, 2019 Yves Chauvin Prize

Aurélie Pirayre, 2018 Yves Chauvin Prize

Olga Vizika-Kavvadias, 2018 Darcy prize awarded by the Society of Core Analysts

In addition, **Hélène Olivier-Bourbigou**, women scientist of the year in 2014, was elected member of the Académie des technologies (French Academy of Technologies) in 2018

Pooled expertise targeting shared research themes

In 2018 and 2019, IFPEN signed a number of fundamental research partnership agreements.

Nationally (in France) with:

ANDRA (French National Agency for Radioactive Waste Management), in the fields of geological modeling, monitoring, instrumentation and analysis, numerical simulations and steel corrosion

the **CNRS**, as a continuation of the collaboration initiated several decades ago in a variety of scientific fields, via research projects, theses and post-doctoral activities undertaken jointly

INRAE (French National Institute for Agriculture, Food and the Environment), focusing on the mobilization of biomass for bioeconomics, biotechnologies and the contribution of soils to the mitigation of climate change

INRIA (French Institute for Research in Computer Science and Automation), in the fields of topological data analysis and automated leaning

Safran Tech, for the development of a joint open source platform in the field of data exploration, optimization and uncertainty processing

Internationally with:

Naples University, on the theme of "chemical engineering – fluidization", with a view to implementing personnel exchanges and setting up collaborative European projects

Stuttgart University, for the NUPUS (interdisciplinary union of porous media research) network

UBC (University of British Columbia), for a partnership focusing on complex fluid flow modeling

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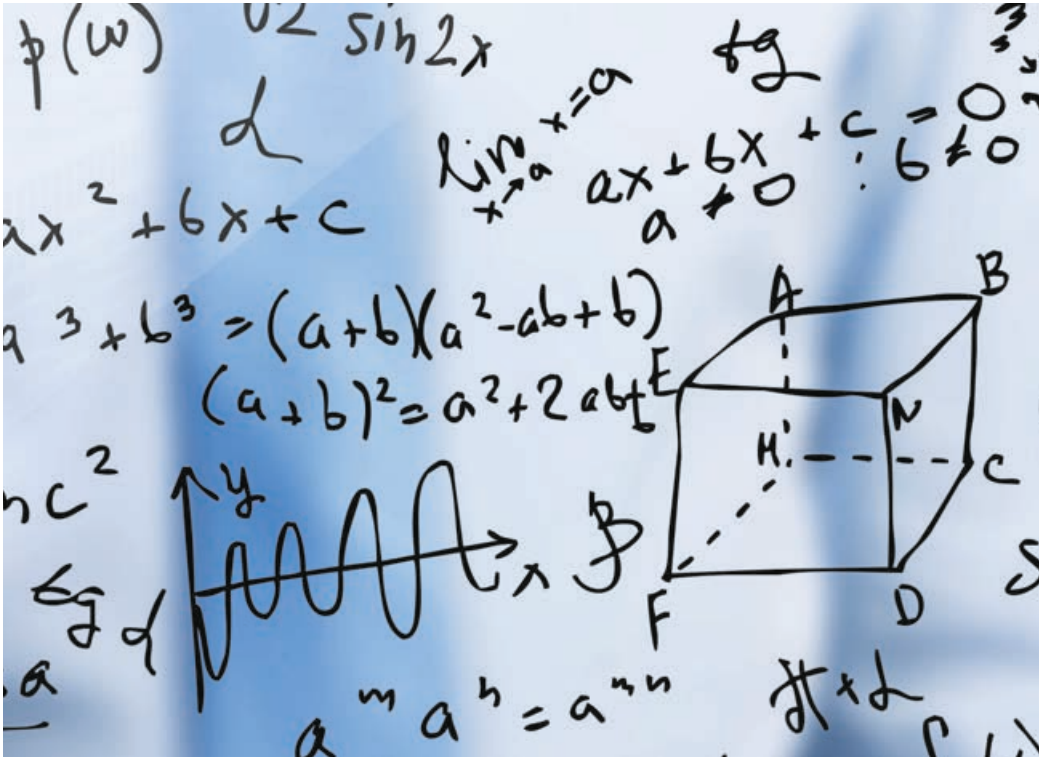

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