Particleworks™
Particle-based simulation software for CAE

users interview

Mitsubishi Chemical Corporation

Analytical modeling for reaction, diffusion, and volatilization in chemical process was finally realized by Particleworks SDK

Mitsubishi Chemical Corporation is a subsidiary company playing a central part under Mitsubishi Chemical Holdings Corporation which is the biggest chemical company group in Japan. It's been developing various business fields contributing widely to society and opening the future, based on the technical foundations which have been developed over a long period mainly in the chemical domain. We have had the pleasure to interview Mr. Yasuharu Kikuchi, a Senior Research Associate of the Process Technology Section, the research and development center in the Kurosaki plant located in Kitakyushu-shi, Fukuoka, to hear the case studies using the MPS based software Particleworks in the evaluation of the chemical process.

Please introduce your business and your role in the research and development center.

Mitsubishi Chemical Holding Group provides 3 business fields, "Performance Products" including high performance products for the information and electronics fields, various resin processed products, film products, and carbon fibers; "Health Care" including pharmaceutical products and diagnosis products; "Industrial Materials" including petrochemicals, carbon products, and industrial gas products. In those fields, Mitsubishi Chemical Corporation has been involved in the "Performance Products" and "Industrial Materials" business fields. To explain some examples in the automotive industry, we produce materials such as polycarbonate used for vehicle headlights and carbon black used in vehicle tires. In addition to such materials and processed products, we also provide batteries and organic EL lights.

In the research and development center, we have proceeded with the research of chemical processes related to the development of those products. Chemical processes mean, briefly, the processes to create products by mixing, reacting, and separating materials of gas, liquid, and solid. For example, materials such as methanol are mixed in a tank, and then it is pumped and put in a reactor vessel. Such reactor vessels are mainly stirring tanks which react materials by mixing with impellers. We conduct research and analysis of the reaction process by mixing, heating, and aerating with various impellers. We've also been working for research and analysis of the crystallization process which precipitate components after crystallization as a chemical separation method in the pharmaceutical field. Additionally, we use simulation technology for predicting phenomena such as, retaining and generation of gas during the product conveyance through the pipes, cooling by using heat exchangers, and excess rectification processes for recycling, to solve problems beforehand and to take measures.

When and for what kind of reasons did you introduce Particleworks?

In the research and development center, we have been using CAD and CAE tools for more than 25 years for a variety of research, and more than 80% of such digital tools are in operation at all times. Because of the chemical processes which always handle fluid

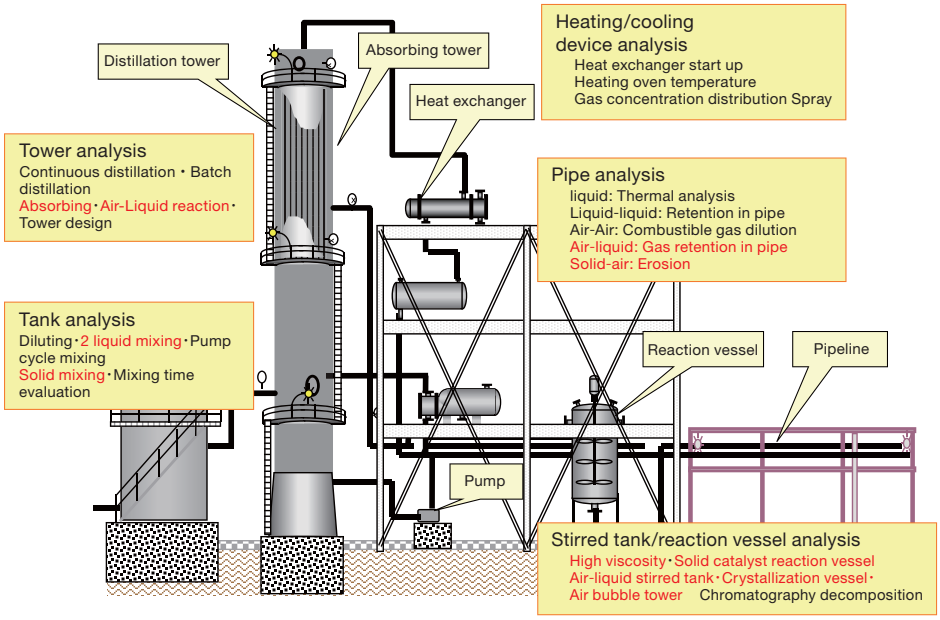

Fig.1 Simulation examples in chemical process

materials, we have used CFD simulation for many years. However, traditional grid method CFD software tools have weak points in that they can't calculate free surface problems with satisfactory shape accuracy of free surface and they can't evaluate the large deformation of the interface well. So, we began to look for a new simulation method and learned about the particle method technology in a society conference. Then we found Particleworks as one commercial software using MPS, one of the particle methods, and finally purchased it about 7 years ago. Thanks to Particleworks supporting GPU computation quickly, we could achieve our goal to improve the calculation costs. Now, 4 engineers of 20 who use CAE tools, are working with Particleworks and 2 or 3 simulation jobs are in operation constantly, which is high usage.

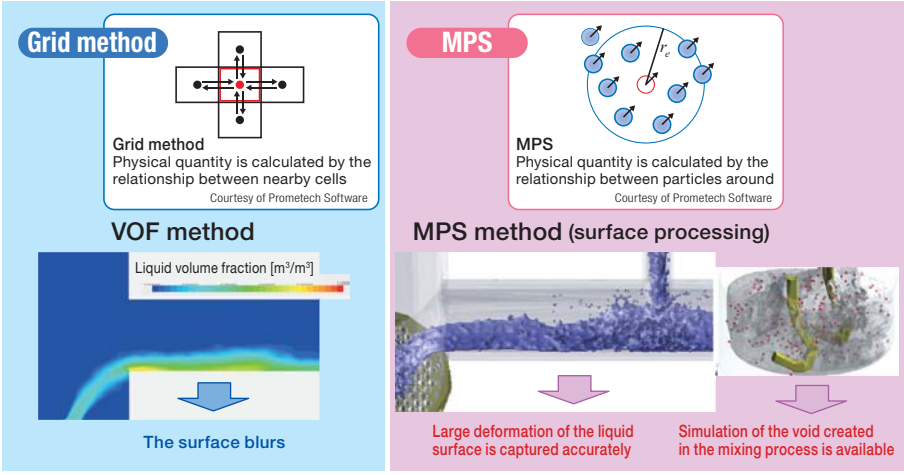

Fig.2 Free surface simulation comparison between grid method and MPS

Could you please give us simulation examples using Particleworks?

Fig.1 shows various simulation examples in the chemical process in our company, and there are relatively more multi-phase problems including air-liquid and solid-liquid. From those examples, we introduce a case study applied to stirring tanks and reactor vessels. Stirring tanks are generally vertical, and they are used to mix mainly low viscosity materials. Impellers are located in vertical stirring tanks and they create boiling, evaporation, bubbles union and division, and phenomenon which the upper interface gets narrow by the rotation in the tanks. A catalyst is used in some cases, and the cases are seen that the solid particles precipitate. The evaluation of those can be simulated by using the grid method CFD software on some level including complicated phenomena, but we take advantage of Particleworks for free surface problems including large deformation. We also use horizontal stirring vessels for some cases when handling high viscosity materials. Thus, we choose suitable stirring tanks and reactor vessels depending on materials viscosity, which are reacted.

In the manufacturing process for polymerization reaction, for instance, the materials at the beginning of the mixing process are low viscosity with 1cP, and they become high viscosity with 10,000P at the end by polymerization reaction. In this case, we use a horizontal reactor vessel for high viscosity, and we didn't have a lot of experience to simulate the process using the grid method CFD software. Because the impellers complex shape makes fluid dynamics complicated and it's very difficult to make simulation model. Also the VOF, one of the grid methods, is generally used for such problems, but VOF can't present interface clearly and the free surface blurs. **Fig.2** is the comparison between the grid method and MPS. We realized that MPS could present the interface very accurately in case the liquid surface deforms dynamically. We also found MPS was very strong for the simulation of horizontal vessels, and had proceeded with the usage of Particleworks.

To specifically explain the reaction process using horizontal vessels, product C and side product D are obtained by the reaction of material A and material B as shown in **Fig.3.** During this process, there is a problem called equilibrium reaction, which is if creating too much C and D, they will be decomposed and return to A and B. Therefore, the reaction doesn't proceed unless the sub product D is removed. So, the impellers in the stirring tank are rotated to remove D, retaining the liquid inside, from the surface to remove it. In actual behavior, the reaction speed is relatively fast, but the removal speed is very slow, because the liquid is high viscosity and the sub product inside isn't removed from the surface quickly. As it's important to encourage the removal, all of the liquid is mixed enough to increase the interfacial area and the mixing performance to encourage the removal. This reaction speed can be measured through experimentation, but it's difficult to know the removal speed. So we had been predicting the approximate speed based on the operation record. Besides, it's not easy to predict how the removal speed will change when using different conditions. So we used Particleworks to evaluate the interfacial area and the mixing performance and succeeded to obtain the removal speed.

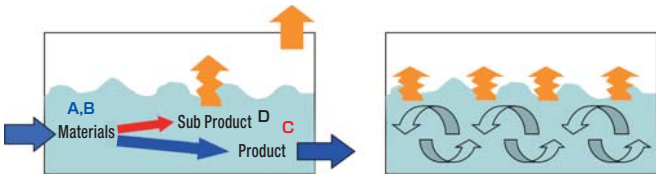

Fig.3 Reaction process by using a horizontal stirring tank

	Initial Concentration	Outside Concentration	Diffusion Coefficient in liquid	Surface Diffusion Coefficient
A	1000	1	1	0.1
B	1000	1	1	0.05
C	1000	1	1	0.02
D	1000	1	1	0.01

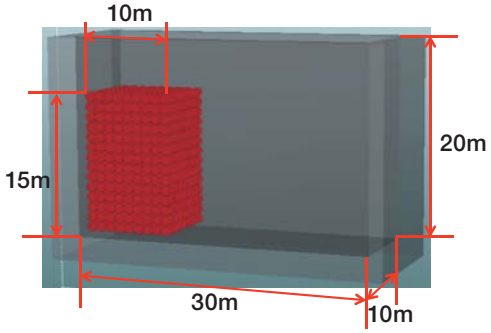

Fig.4 Parameters for the dam break problem

What kind of simulations do you use the software development kit SDK for?

Although MPS is superior in terms of capturing the interfacial area accurately, only the standard capabilities of Particleworks couldn't calculate how the sub product D was removed. So, we decided to use Particleworks SDK, the software development kit, and had considered analytical modeling of reaction, diffusion, and volatilization in the stirring tank. As the way of modeling in SDK, the equation of component X concentration is expressed by 3 source terms of solution which are diffusion, volatilization from surface, and reaction. The same equation in Particleworks was used for the diffusion Laplacian. We used the equation of the chemiosmotic hypothesis for the volatilization from surface, and used the Particleworks free surface judgement and interfacial area calculating formula for the interfacial area. Regarding the calculation of the reaction, we used the chemical equation written in common text.

We had examined if the model for reaction, diffusion, and volatilization worked correctly by using the dam break problem shown in **Fig.4.** Here, 4 components of A, B, C, and D were set, the initial concentrations inside and outside were defined as the same, and only the diffusion coefficient was changed to see the tendency. The initial distance between particles was set at 1m. At the beginning, we validated the diffusion model. Like **Fig.5** shows, the liquid flowed rapidly by the dam break, and the component inside diffused gradually, so we could confirm the model was created correctly.

Then we evaluated the reaction model. Seeing the transformation of component A, for example, the concentration of A decreased as time proceeded, which is shown in **Fig.6.** And finally the concentration increased again like we can see that the color returned to orange. This is the equilibrium reaction which was explained before.

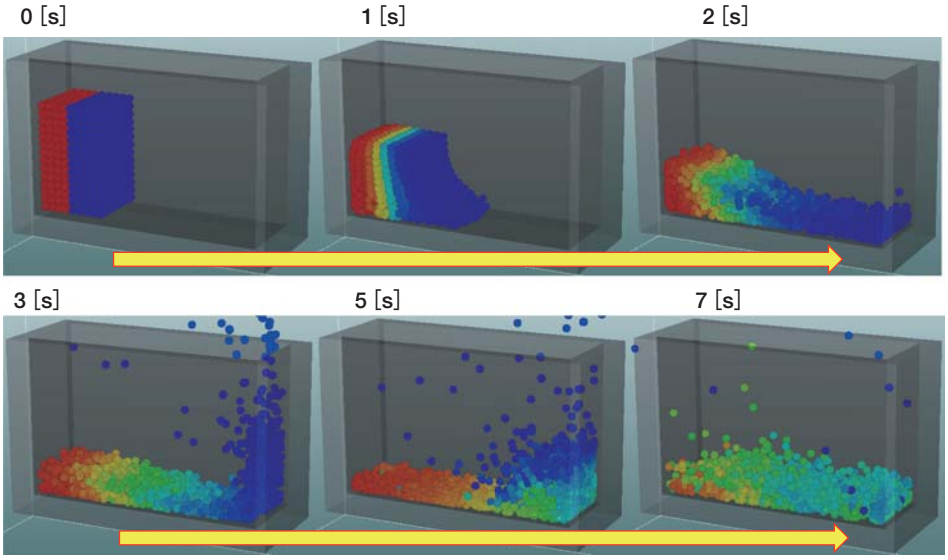

Fig.5 Time dependent change of the diffusion model concentration for A

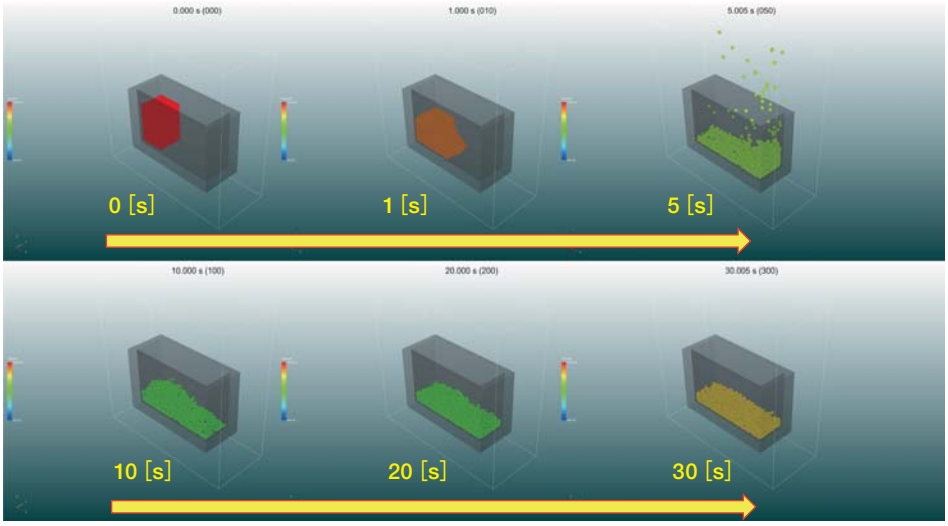

Fig.6 Time dependent change of the reaction model concentration for A

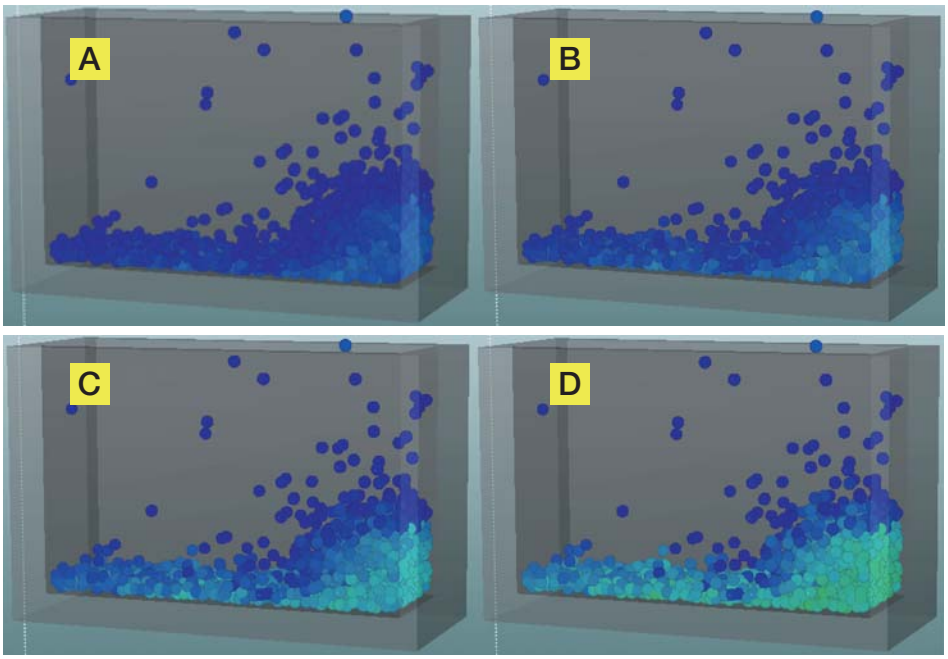

Fig.7 Time dependent change of the volatilization model concentration for A (after 5s)

The theoretical result was obtained by hand calculation as the reaction formula was simple, and it corresponded to the simulation result well and we could know that the reaction model was created correctly. Finally, we evaluated the volatilization model. By defining different diffusion coefficients for A, B, C, and D, we changed the degree of volatilization. Like the results shown in **Fig.7,** especially D is easier to understand, the surface concentration is low and the inside concentration is still high. So we could understand that the component was removed only from the surface and the volatilization was modeled correctly.

It seemed there was no problem so far, but in fact we found that the volatilization occurred after 1 second near the wall which should not be an interface. It happened because of the problem that the interfacial area was calculated near the wall after 0.1 second. Besides, the interfacial area was wider than the theoretical result at the steady state level, and we also realized a problem that there is a gap in the interfacial area calculation, which was important for volatilization. Later, we knew that it occurred by the default free surface judgement parameters and the calculation way, so we asked Prometech for help and improve it by changing the calculation way of the interfacial area. After making some improvements on the free surface judgement and calculation using a different equation from a standard pressure calculation, we could obtain the result which almost corresponded to the theoretical result, and finally, the way we choose was evaluated as enough to use.

There are many multi-fields problems in chemical processes and there are numerous opportunities to use MPS, but in fact there are still some cases that we can't evaluate enough by the standard capabilities of Particleworks. However, the analytical modeling of special phenomena such as reaction, diffusion, and volatilization became realized by using SDK, and we could go forward with our research.

Could you please tell us the future vision about your research and the simulation activities, and expectations of Prometech?

Yasuharu Kikuchi,
Senior Research Associate,
Process Technology Section,
R & D Center

In the future, regarding the applications to our practical business, we would like to use Particleworks with problems of kneading and diffusion which Lagrangian method is effective for, solid and fluid combinations, and free surface problems including large deformations by utilizing our experience so far. We think that visualization and realization of phenomena accelerate our research, so we would like to positively use Particleworks more. With respect to the capabilities, we have requirements for model, accuracy, HPC, and pre/post processor. So we look forward to Prometech in developing the software step by step with users including us.

Thank you very much for your valuable input. Mitsubishi Chemical Corporation is one of the users which began to use Particleworks from the early period and has provided lots of useful ideas for our software development. We'd like to grow further by receiving such ideas in the future, too. Again thank you for cooperating with the interview despite your busy schedule. Prometech will continue to provide further support for your better product development.

Reference
Prometech Simulation Conference 2015 presentation material

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Mitsubishi Chemical Corporation

Head Office: Chiyodaku, Tokyo
Founded: August, 1933
Activities: Performance Products (Information electronics, Performance chemicals, Batteries), Industrial Materials(Petrochemicals, Carbons,Polymers)
URL: https://www.m-chemical.co.jp/en

Particleworks™
Particle-based simulation software for CAE

Particleworks is a CFD software based on an advanced numerical method known as the Moving Particle Simulation (MPS) method. The mesh-free nature of MPS allows for robust simulation of free-surface flows at high resolutions, saving the need to generate meshes for the fluid domain.

Contact

PROMETECH.
Prometech Software, Inc.
Head Office
Hongo Dai-ichi Building, 8th Floor, 34-3,
Hongo 3-chome, Bunkyo-ku, Tokyo 113-0033, Japan
Tel: +81-3-5842-4082 Fax: +81-3-5842-4123
West Japan branch office
Asahi Kaikan, 7F, 3-3, Sakae 1-chome,
Naka-ku, Nagoya, Aichi 460-0008, Japan
Tel: +81-52-211-3900 Fax: +81-52-211-3901
URL: www.prometech.co.jp
E-mail: sales@prometech.co.jp