

Computer Simulation of a Novel Photocatalytic Reactor Using Distributive Computing Environment

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In this paper, the numerical simulation for the *in situ* degradation of toxic water pollutants in the presence of semiconductor catalyst particles is considered. The computer simulation is in search of an efficient photocatalytic reactor design to achieve better fluid-catalyst contacting to minimize mass transfer limitation. In addition, in the present work, a state-of-the-art efficient computational technique, namely, distributed computing, has been employed to expedite the speed of calculation and overcome the memory bottleneck present in a single workstation. A comparative study has also been made of the computational effort required for a serial, parallel and distributed computing environment. The results show that the distributed computing technique is an economical and efficient method for overcoming difficulties, such as the memory bottleneck present in single workstations and the long computation time, associated with computer simulations of reacting flows.

1 Introduction

Reactive flow modeling is an excellent tool for enhancing the performance of any process vessel. Applying such a technique to reactors can be especially fruitful because of the reactors' central role in chemical processes. In most reactor design situations, the reactions and the catalysis system are set beforehand. For any given combination of them, reactor performance becomes a complex function of the underlying transport processes. These in turn are governed by the fluid dynamics of the reactor. Detailed flow analysis and modeling can, accordingly, lead to numerous performance improvements of reactors by identifying and getting rid of any fluid maldistribution inside the reactor, thereby improving selectivity and capacity of the reactor.

Computational fluid dynamics (CFD), which solve fluid dynamic problems with the aid of a digital computer, offer many advantages. With CFD, the engineer can build a flow model having global and local information alike, simulating the flow and turbulence characteristics of reactors. CFD models may well be the only good tools available for studying the fluid dynamics as they require relatively few restrictive assumptions and give a complete description of the flow field even for complex configurations. In this paper, numerical simulation for *in situ* degradation of toxic water pollutants in the presence of semiconductor catalyst particles is considered. The computer simulation is to explore an efficient photocatalytic reactor design to achieve better fluid-catalyst contacting to minimize mass transfer limitation, and simultaneous increase of flow rate to increase water treatment capacity by the reactor and residence time of the pollutant inside the reactor for enhancement of yield.

In this paper, a state-of-the-art efficient computational technique was employed to expedite the calculation and overcome the memory bottleneck present in single work-

stations. In recent years, technology has been shifting from the single mainframe to distributory networks where powerful computers are linked by high-speed local communication networks to form workstations. Unlike normal computers, which do calculations sequentially, parallel computers break up a task into parts and then perform them simultaneously on a powerful machine that has a single cabinet with multiple CPUs connected to a large set of computers. Distributed computing differs from parallel computing in the sense that a set of computers connected by a network are used collectively to solve a single large problem by distributing the load among all the processors.

2 Photocatalytic Reactor

The increasing level of global industrialization has led to the increase of water pollution. Harmful impurities present in water supplies and in the discharge of wastewater from chemical industries, power plants and agricultural sources call for an efficient and economical method of destroying the toxic compounds present in them. For years, engineers have relied on a variety of traditional water treatment processes that include phase transfer, biological treatment and chemical treatment by a combination of ozone, hydrogen peroxide and/or high-energy ultraviolet light. All these existing water treatment processes currently in use have limitations. Phase-transfer methods remove unwanted pollutants from wastewater but they do not eliminate the pollution problem entirely, whereas in biological treatment some of the toxic compounds present are found to be lethal for microorganisms intended to degrade them. Although processes based on aqueous-phase hydroxyl radical chemistry [1] are becoming powerful oxidation methods that can destroy toxic organic compounds present in water, all the present chemical treatment processes either use high-energy ultraviolet light or strong oxidants of serious hazardous and therefore undesirable nature [2]. Moreover, selection of operating process parameters is very much dependent on the type of pollutants present [3]. Furthermore, several intermediates, at times of more hazardous nature, are formed in these processes and because of very low efficiencies,

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overall treatment cost becomes high if destruction of intermediates and complete mineralization are to be achieved [4].

Heterogeneous photocatalysis [5] is one of the advanced oxidation processes that couple low-energy ultraviolet light with semiconductors acting as photocatalysts, and it has emerged as a viable alternative for solving environmental problems overcoming many of the drawbacks that exist for the traditional water treatment methods [6]. In this process, *in situ* degradation of traces of organic substances is achieved, and it has promoted much research activity in various groups around the world in recent years. The appeal of this process technology is the prospect of complete mineralization of the pollutants into environmentally harmless compounds. The carbon-containing pollutants are oxidized to carbon dioxide and water, while the other elements bonded to the organic compounds are converted to anions, such as nitrate, sulfate or chloride. Practically any organic pollutant can be completely mineralized by this process into harmless substances and include aliphatics, aromatics, polymers, dyes, surfactants, pesticides and herbicides [7].

Activation of the catalyst is achieved by electron-hole pair formation initiated through the absorption of a photon of ultraviolet bandgap energy [8]. Excited-state conduction band electrons and valence band holes may recombine and dissipate the input energy as heat or they may become separated and involved in electron transfer reactions with species in the solution the material is immersed in. In the presence of suitable scavengers or surface defects they become trapped and subsequently enter into redox reaction with species adsorbed on the surface or present within the electrical double layer of the charged particles. The holes react with electron donors, for example, hydroxyl ions or water, to form hydroxyl radicals. The electrons, on the other hand, react with an electron acceptor, for example, molecular oxygen. Of all the different semiconductor photocatalysts tested, TiO₂ appears to be the most active [9]. The anatase form of TiO₂ requires photons having energies greater than 3.2 eV ($\lambda < 380$ nm) to initiate bandgap excitation. It satisfies the foremost criteria for degradation of organics as the bandgap domain of the catalyst lies within the redox potential of the H₂O/OH[•] (OH⁻ → OH[•] + e⁻; E° = -2.8 V) couple. Moreover, TiO₂-based photocatalysis is more appealing than the other conventional chemical oxidation methods because the catalyst is cheap, biologically and chemically inert, insoluble under most conditions, photostable, nontoxic, the reaction rate is relatively high if a large catalyst surface area is provided, and it can be used for an extended period without substantial loss of its activity. More importantly, it requires only about 1 W/m² light [10] and can even be activated by sunlight [7].

2.1 Major Problems in the Photocatalytic Reactor Development

In spite of the potential of this promising technology, the development of a practical water treatment system has not yet

been successfully achieved. In the last few years, a large number of publications [2–7] have appeared based on laboratory-scale studies with generally positive results for very diverse categories of toxic compounds in water. However, technical development to pilot-scale level has not yet been successfully achieved although there are numerous patents world-wide. None of these has been successfully brought out of the laboratory yet.

There are several factors that impede the efficient design of a photocatalytic reactor [11]. In this type of reactor, besides the requirement of good contact between reactants and catalysts, it is also necessary to achieve an efficient exposure of the catalyst to light irradiation. In fact, in a photocatalytic reactor, besides conventional reactor complications, such as mixing, mass transfer, reaction kinetics, catalyst installation, etc., an additional engineering factor related to catalyst illumination becomes relevant. The problem of photon energy absorption has to be considered regardless of reaction kinetics mechanisms. The high degree of interaction between the transport processes, reaction kinetics and light absorption leads to a strong coupling of physicochemical phenomena and no doubt, this is the major obstacle in the development of a photocatalytic reactor. The illumination factor is of utmost importance since the amount of catalyst that can be activated determines the water treatment capacity of the reactor.

In numerous investigations, an aqueous suspension of the catalyst particles in immersion- or annular-type photoreactors has been used. Depending on the means of agitation, the photoreactor resembled that of slurry or fluidized-bed reactors. However, the use of suspensions requires the separation and recycling of the ultrafine catalyst from the treated liquid which is usually an inconvenient, time-consuming and expensive process. Moreover, the depth of penetration of UV light is limited because of the strong absorption by catalyst and dissolved pollutants. One solution to the above problem is to immobilize the catalyst onto a fixed transparent support [12]. The immobilization of the catalyst, however, generates a unique problem. The reaction occurs at the liquid-solid interface and in some cases, the overall rate may be limited to mass transport of the pollutant to the catalyst surface. In addition, the rate of reaction is usually slow because of the low concentration level of the pollutant and therefore, there is a need for high values of illuminated catalyst density, the amount of active catalyst surface in contact with the reaction liquid treated inside the reactor. The development of a reliable knowledge base is still in its initial stages related to the catalyst preparation and its activation, chemistry and kinetic networks of the pollutant degradation, intrinsic reaction kinetics that at times is mass transfer-controlled, the process of photon energy absorption, and reactor design.

2.2 Basic Design Concept of the Present Reactor

One major barrier to the development of a photocatalytic reactor is that the reaction rate is usually slow compared to

conventional chemical reaction rates, due to low concentration levels of the pollutants. Another crucial hurdle is the need to provide large amounts of active catalyst inside the reactor. Although the effective surface area of the porous catalyst coating is high, only a thin coating (about 1 μm thick) can be applied to a surface. Thus, the amount of active catalyst in the reactor is limited and, even if individual degradation processes can be made relatively efficient, the overall conversion efficiency will still be low. This problem severely restricts the processing capacity of the reactor, and the time required to achieve high conversions is measured in hours, if not in days.

For large-scale applications, reactor configurations must address two most important parameters, namely, uniform light distribution inside the reactor and high surface areas for catalyst coating per unit volume of reactor [11]. New reactor design concepts must provide a high ratio of activated immobilized catalyst to illuminated surface and require a high density of active catalyst in contact with the liquid to be treated inside the reactor. The only way to overcome the above deficiencies inherent in conventional photocatalytic reactor designs is either by using an immersion-type reactor with very narrow diameter tube lamps [13] or by a distributive-type of photocatalytic reactor design in which the catalyst is fixed to a structure in the form of hollow glass tubes [14]. The design based on hollow glass tubes allows for a much higher illuminated surface area per unit reactor volume whereas the other design provides much higher values for the active catalyst surface area, and the catalyst can be activated uniformly at its highest possible level [15]. An experiment performed has shown a very promising result [16], but the overall destruction rate was limited to mass transport of the pollutant to the catalyst surface [17]. The reaction occurs at the liquid-solid interface, and mass transfer from the bulk of the liquid to the catalyst surface plays an important role in the overall rate of pollutant destruction [10].

3 Computer Simulation

The increase in reactor efficiency over a conventional photocatalytic reactor was in spite of the fact that the design of the test reactor was far from optimum with respect to mass transfer, flow distribution and efficiency of packing of the tube lamps inside the reactor [13]. Computer simulation is used to fine-tune the reactor design to achieve better fluid-catalyst contacting to minimize mass transfer limitation.

The reactor considered in the simulation consists of a cylindrical vessel (diameter 0.05 m, length 0.25 m) within which 7 hollow tubes (diameter 0.006 m) coated on its peripheral surface with catalyst were placed in staggered manner with 0.006 m pitch (Fig. 1). The reactor resembles that of a shell and tube heat exchanger with the reaction liquid flowing through the shell-side over the outside surface of the catalyst-coated hollow tubes. The liquid was intro-

duced and collected through an inlet and outlet port placed tangentially to achieve greater mixing and minimizing dead zones. The effective illuminated catalyst surface area and the volume of the reactor are $3.3 \times 10^{-2} \text{ m}^2$ and $4.9 \times 10^{-4} \text{ m}^3$, respectively. The parameter, κ , defined as total illuminated catalyst surface area that is in contact with the reaction liquid per unit volume of the liquid treated in the reactor volume is equal to $75 \text{ m}^2/\text{m}^3$.

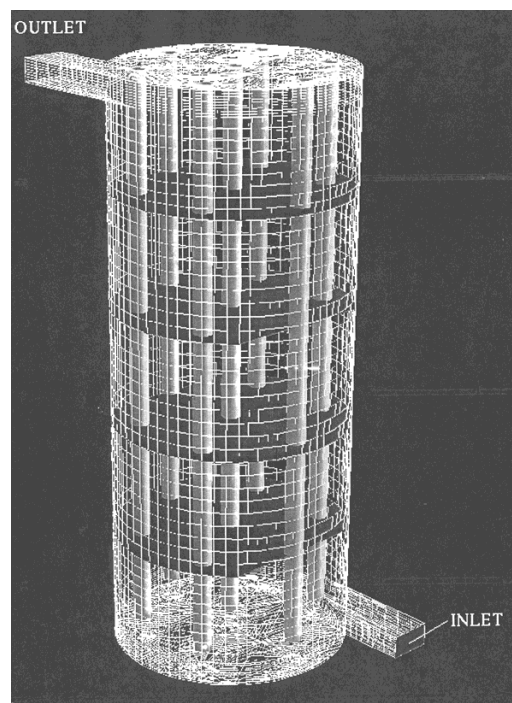


Figure 1. Reactor configuration and computational domain of the reactor for computer simulation.

Numerical simulation of the reactor is performed using a commercial CFD package FLUENT/UNS to determine effects of flow rates, diffusion coefficients, reaction rate constants and inter lamp spacing. The application of CFD to reactors entails a number of tasks: (a) formulating the relevant transport equations, (b) establishing the necessary constitutive and closure equations, (c) formulating appropriate boundary conditions, (d) selecting the most suitable numerical techniques to solve the equations, (e) choosing (or developing) a suitable computer code to implement the numerical techniques, and (f) developing effective flow simulation strategies.

In order to obtain accurate results, the 3-D model of the reactor was divided into control volumes ranging from 500.000 to 1.000.000 cells distributed unevenly in the computational domain. Computation had to be carried out for at least 2000 iterations for convergence, which may require a couple of days on a single SGI workstation. In the wake of this, the present work employs a state-of-the-art computational technique, viz., distributed computing, to expedite the calculation and overcome the memory bottleneck present in single workstations.

3.1 Computational Aspects: Parallel Processing on a Distributed Computing Environment

Distributed computing leads to what is known as the "parallel virtual machine" (PVM), and it differs from parallel computing in the sense that the former is a process whereby a set of computers connected by a network are used collectively to solve a single large problem. Parallel computing, on the other hand, is the process of solving large problems on a powerful machine that has a single cabinet with multiple CPUs connected to a large set of memory. As more and more organisations have high-speed local area networks interconnecting many general-purpose workstations, the combined computational resources may exceed the power of a single high-performance computer. As the distributed computing exploits a collection of networked computers, a user may have to contend with several different types of heterogeneity: architecture, data format, computational speed, machine load and network load.

3.1.1 Heterogeneous Network Computing

Architecture: The set of computers that makes the parallel virtual machine may be composed of a wide range of architecture types, such as 386/486 PC class machines, high performance workstations, shared memory multiprocessors, vector supercomputers, and even large MPPs.

Data Format: Different architectures offer data incompatibility which is an important point in distributed computing because data sent from one computer may be unreadable on the receiving computer.

Computational Speed: Even if the set of computers in the virtual machine are all workstations with the same data format, as in our case where all are SGI machines, there is still heterogeneity due to different computational speed. Tab. 1 shows the configuration of the machines used in the present research.

Table 1. Configuration of workstations that make up the parallel virtual machine at any time.

Compute node (SGI machines)	Number of CPUs	Memory (Mbytes)	CPU speed (MHz)
Puma	1	128	250
Leopard	1	96	250
Inxz5	1	64	250
Inxz4	1	64	133
Inxz3	1	64	133
Panther	4	256 (total)	200 (each)

Machine Load: The problem of computational speed can be very subtle as the networked computers can have several other users on them running a variety of jobs, the machine load can vary dramatically. The result is that the effective computational power across identical workstations can vary by an order of magnitude.

Network Load: Like machine load, the network load imposed by other network users, who may not even be using any of the computers in the virtual machine, will have a strong effect on the time taken to send a message over the network. This sending time becomes important when a task is sitting idle waiting for a message, and it is even more important when the parallel algorithm is sensitive to message arrival time.

It is important to be aware that heterogeneity can appear dynamically even in simple setups. Despite these numerous difficulties caused by heterogeneity, distributed computing offers many advantages. It allows one to use existing hardware and the cost of computing can be very low. The virtual computer resources can grow in stages, take advantage of the latest computational and network technologies.

Simulation of the complex and computationally intensive physicochemical phenomena using the distributed computing technique expedites the progress of the present research in many ways. The time taken to produce the desired result has plummeted from days to hours. Besides this speedup, the visualization of the data plays a crucial role in the final analysis, and for this purpose powerful SGI machines were used. The results show that the distributed computing technique is the most economical and efficient method for overcoming difficulties, such as the memory bottleneck present in single workstations and the long computation time, associated with computer simulations of reacting flows.

3.2 Distributed Computing in Fluent/UNS

Fluent/UNS was used for solving the present compute-intensive problem in parallel on a distributed computing environment. In order to use the parallel version of the Fluent/UNS, the grid was partitioned into multiple subdomains such that the number of partitions was an integral multiple of the number of compute nodes available (e.g., 8 partitions for 1, 2, 4, or 8 compute nodes). Each partition (or group of partitions) then resides on a different node. These compute nodes may be on a massively parallel computer, multiple-CPU workstation, or a network of heterogeneous workstations. In general, as the number of compute nodes increases, the turnaround time for the solution will decrease. However, parallel efficiency decreases as the ratio of communication to computation increases. Hence, the granularity of the large problem is an important factor.

Partitioning was done with the serial version of Fluent/UNS, and then it was read into the parallel solver. The partitioning of the grid was executed with three major goals: (a) creating partitions with equal numbers of cells, (b) minimizing the number of partition interfaces, i.e., decreasing the partition boundary surface area, and (c) minimizing the number of partition neighbors. Balancing the partitions (equalizing the number of cells) ensures that each processor has an equal load and that the partitions will be ready to communicate at about the same time. Since communication between partitions is a relatively time-consuming process, minimizing the number of

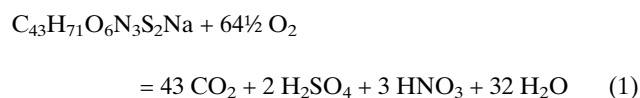
interfaces reduces the time associated with this data interchange. Minimizing the number of partition neighbors reduces the chances for network and routing contentions. In addition, minimizing partition neighbors is important on machines where the cost of initiating message passing is expensive compared to the cost of sending longer messages. The partitioning scheme in Fluent/UNS uses a recursive bisection algorithm to create the partitions and has no limitations on the number of partitions. The coarse grid created for the multigrid convergence acceleration was confined within the partitions; that is, the coarse grids did not cross partition boundaries.

4 Results and Discussion

4.1 Reacting Flow

Initially, a reasonably converged solution was obtained for the velocity and pressure equations. The conservation equations were solved in Fluent using RNG (re-normalized group) k - ϵ model. The reaction part of the solver was then activated, and using the almost converged solution as the initial condition, a complete solution of the reacting flow model was obtained. The converged velocity profiles at various regions of the reactor were observed to determine the degree of mixing (Fig. 2). Fluid mixing was used as one of the important criteria in the efficient design of a photocatalytic reactor, as the transport of reactants from the bulk of the liquid to the catalyst surface determines the extent of fluid-catalyst contacting and overall conversion. The velocity profile shows that maximum mixing takes place at the bottom of the reactor where the fluid enters the reactor tangentially with a swirling motion. There is also a good degree of mixing in the mid-region between the inlets and outlets.

The advantage of using computer simulations is that the length of the reactor required for the complete degradation of a particular pollutant can be determined readily, compared to time-consuming expensive experimental studies. In addition, the flexibility of determining the effects of various process parameters in computer simulations will be useful, particularly flow rates, as the degradation rate strongly depends on the residence time of the fluid inside the reactor. A typical case of degradation of a textile dye pollutant, Special Brilliant Blue, $C_{43}H_{71}O_6N_3S_2Na$, and formation of carbon dioxide is shown in Figs. 3a and 3b. The stoichiometric equation that represents the chemical reaction for the present study is:



The figure shows that most of the dye pollutant can be degraded when the Reynolds number is about 2000, thereby indicating that the reactor could be used for treating a larger capacity if mixing is improved.

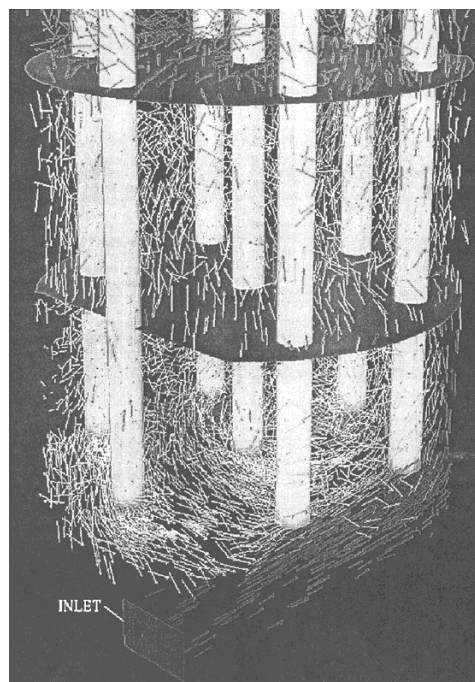


Figure 2. Velocity vectors showing the degree of mixing in the reactor.

Fig. 4 shows the effect of various parameters on the conversion the dye pollutant. As the flow rate was increased, conversion decreased since the residence time of the pollutant decreased. However, the capacity of the reactor will be low when a slow flow rate is used. When the reaction rate constant was increased beyond $0.1 \mu\text{mol}/\text{m}^2/\text{s}$, conversion did not improve much, implying that the overall rate is not controlled by reaction kinetics. When the reaction rate constant was reduced to $0.001 \mu\text{mol}/\text{m}^2/\text{s}$, a factor of 100, conversion decreased only by 1.4%, confirming that overall reaction is mass transfer-controlled. This is further justified when the diffusion coefficient was varied keeping other parameters fixed at the reference value. Diffusion coefficients of the pollutant in the aqueous phase are normally of the order of $1.0 \times 10^{-9} \text{m}^2/\text{s}$, and Fig. 4 reveals that conversion is controlled by the diffusion of the pollutant from the bulk to the catalyst surface. This was further confirmed by varying the intertube spacing. By reducing the pitch one would reduce the distance a species has to travel to come in contact with the catalyst surface. Hence, conversion will increase with the decrease of tube clearance, particularly when the flow is laminar as there is no mixing of fluid particles. The effect was more pronounced at a smaller pitch (34.3% decrease in conversion when the pitch was increased from 0.003 to 0.004 m), while a drop in conversion is less noticeable when lamp spacing is large (only 15% drop when the pitch was increased from 0.006 to 0.007 m).

Fig. 4 reveals the importance of diffusion in the design of a photocatalytic reactor. Conversion is primarily controlled by the flow and diffusion of a pollutant and is practically independent of the reaction rate. When the diffusion coefficient is very low, low flow together with smaller intertube spacing must be used to ensure high conversion.

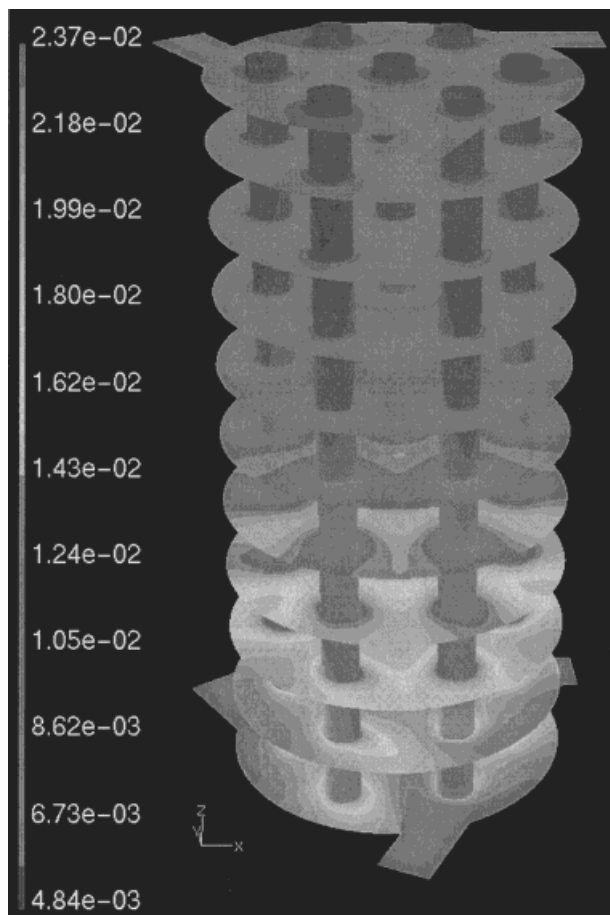


Figure 3a. Degradation of dye pollutant in the photocatalytic reactor. Flow direction is from bottom to top.

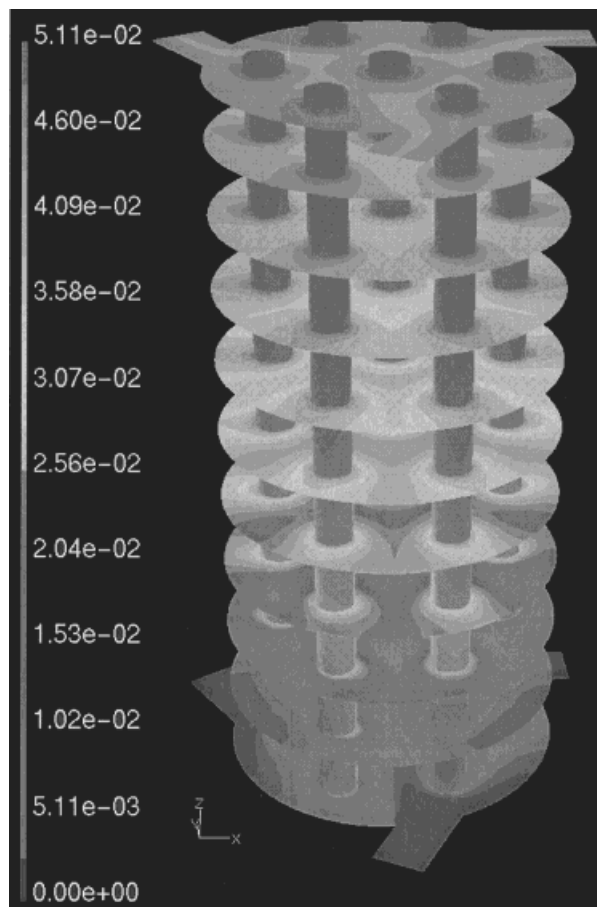


Figure 3b. Formation of carbon dioxide in the photocatalytic reactor. Flow direction is from bottom to top.

However, a low flow rate results in a low throughput. Creating turbulence enhances fluid mixing in the reactor, thereby conversion improves. However, if turbulence is generated only by increasing the flow rate, the residence time of the

pollutant in the reactor will decrease and conversion will decrease subsequently. Therefore, one must find an optimal flow rate first and then maximize both fluid mixing and residence time of the pollutant in the reactor by introducing baffles and selecting proper reactor configurations.

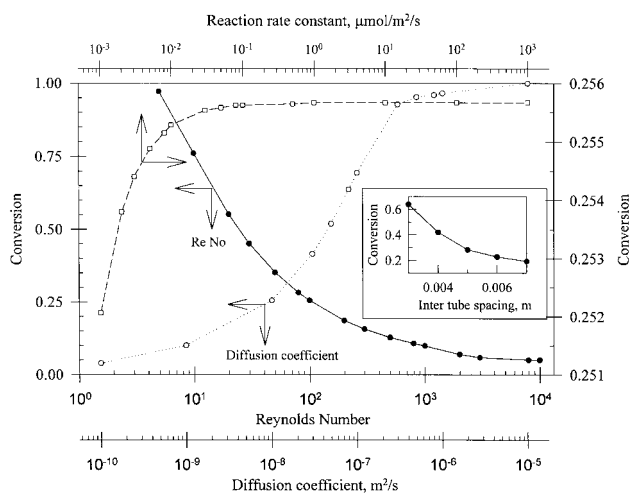


Figure 4. Effect of Reynolds number, mass diffusivity, reaction rate constant and tube pitch on the conversion of the dye pollutant (reference values: Reynolds number, $Re = 100$, mass diffusivity, $D = 10^{-8} \text{ m}^2/\text{s}$, reaction rate constant, $k = 0.1 \text{ } \mu\text{mol}/\text{m}^2/\text{s}$, pitch, $P = 0.006 \text{ m}$).

A comprehensive computer simulation on the design of the reactor is currently carried out using distributive computing to expedite the calculation of coupled nonlinear PDEs and overcome the memory bottleneck present in a single workstation. The advantage of using computer simulations is that the length of the reactor required for the complete degradation of a particular pollutant can be determined easily compared to time-consuming expensive experimental studies. The result can then be verified experimentally.

4.2 Computational Results

The present model solves not only the transport equations (pressure and u, v, w -momentum) but also six species of conservation equations. When the turbulence model is activated, additional two equations (for k and ϵ) need to be solved. For an accurate solution, these twelve highly nonlinear and coupled equations are solved at each cell (a total of more

than 600.000 cells) for each iteration. This type of computation demands very high memory and cpu speed, which normally exist in expensive parallel supercomputers. However, supercomputers may not always be available and even if they are available, the software may not be available on them and one may have to look for alternatives.

In this paper, up to a maximum of five SGI workstations (compute nodes) with different types of configurations were interconnected to act as a single virtual machine, hence the name "parallel virtual machine". The computational domain was divided with respect to the total number of workstations available. Tab. 2 shows the typical distribution of cells when a relatively *coarse* grid (127.062 cells) was partitioned into four subdomains. It can be seen that the number of cells in each subdomain was almost equal to provide an even load on all the four workstations that make up the virtual machine. The memory required at each compute node is also shown in the table and can be compared with Tab. 1 to see the available physical memory at any compute node that would eventually make the virtual machine.

Table 2. Typical domain decomposition and the memory required at each compute node.

Compute node	Number of cells	Memory used
Puma	31759	41 Mbytes
Leopard	31774	41 Mbytes
Inxz5	31761	41 Mbytes
Inxz3	31768	41 Mbytes

The performance of the virtual machine is usually measured by means of two parameters: *speedup* and *efficiency*. The speedup, S_p , is defined as the ratio of the wall clock time of the single workstation (running a serial version), t_w , to the wall clock time of p compute nodes that make up the virtual machine, t_p :

$$S_p = \frac{t_w}{t_p} \quad (2)$$

The efficiency, E_p , is the ratio of the speedup to the total number of processors (compute nodes) used:

$$E_p = \frac{S_p}{p} \quad (3)$$

The wall clock times of 60 iterations for various virtual machine configurations are shown in Tab. 3 for the case of 127.062 cells mesh. A single workstation (*Puma*) takes about 113 minutes and the total memory (164 Mbytes) required exceeded the physical memory (128 Mbytes) of the computer. In this case, part of the program will have to be swapped (using the swap space) in and out of the hardisk. Swapping data between the hardisk and physical memory can be very time-consuming. This was reflected in the case when the domain

was partitioned into two subdomains and solved on two compute nodes (*Puma* and *Leopard*) in parallel using the distributed computing technique. The total wall clock time taken was only about 53 minutes which gives a speedup of 2.13 with an efficiency of about 1.066. In reality, the speedup and efficiency should not exceed 2.0 and 1.0, respectively, as additional time would be required for communication between the nodes. This high speedup value can be explained in terms of the memory required at each compute node. When the domain was partitioned into two subdomains, each subdomain required less memory, less than the physical memory of the two machines, to carry out the computation. Hence, there was no need to use the swap space of the machines and much time was saved. The result shows the interesting fact that distributed computing is an efficient alternative to big swap space. For the case of a virtual machine with three compute nodes (*Puma*, *Leopard* and *Inxz5*), the time required to do the same 60 iterations was only 37 minutes as compared to 113 minutes on a single workstation. This gives a speedup of 3.054 and an efficiency of 1.018. Once again, the results show that the distributed computing method of utilizing the distributed memory of a workstation cluster is very economical for the cases of large problems where the swap space may have to be used when solved on a single machine.

Table 3. Distributed computing performance for various configurations of virtual machines. The times shown are the wall clock time.

Number of compute nodes	Time (minutes)	Sp	Ep	Number of users
1	113	1.000	1.000	0
2	53	2.130	1.066	0
3	37	3.054	1.018	0
4	46	2.520	0.630	3
4 (Panther)	44	2.570	0.643	4
5	40	2.860	0.565	3

The domain was further partitioned into four subdomains and solved on a virtual machine made up of four workstations (*Puma*, *Leopard*, *Inxz5* and *Inxz3*). The time taken was about 46 minutes, which gives a speedup of 2.52 with an efficiency of 0.630. The computation is still much faster as compared to the case of a single workstation. The values of speedup and efficiency were relatively much lower and this is expected as there were other users logged on to the workstations that made up the virtual machine. The computation with other users logged on to the virtual machine was deliberately done to obtain a realistic distributed computing environment. In addition, the communication time was also increased with increasing number of compute nodes. The same problem was

then solved on *Panther*, a 4-CPU multiprocessor with shared memory configuration. The time required for 60 iterations was about 44 minutes, giving a speedup of 2.57 with an efficiency of 0.642. The number of users logged on to *Panther* were four compared to three on the four-node virtual machine. It is also important to note that three of the four machines that make up the virtual machine have a higher CPU speed (250 MHz) as compared to the CPUs of *Panther* (200 MHz). Comparing the results, speedup and efficiency, of the shared memory configuration of *Panther* to the distributed memory configuration (four-node virtual machine), the difference is only marginal. This shows that an existing cluster of multipurpose workstations can be interconnected to form a virtual machine that is as powerful as a single cabinet multiprocessor, which could be very expensive.

Finally, the domain was divided into five subdomains and solved on a five-node distributed computing environment. The total time taken, with three other users logged on, is only about 40 minutes for 60 iterations, which gives a speedup of 2.86 with an efficiency of 0.565. Although the savings in time may not seem very high as compared to the previous case of four machines (44 minutes), the final solution requires almost 2000 iterations on a much finer grid (more than 500.000 cells), and the overall ultimate savings can be very high. It is also important to be aware of the fact that the final solution, with large subdomains, will have a high computation-to-communication time ratio, resulting in a more efficient virtual machine with good speedup.

5 Conclusions

Heterogeneous photocatalysis on semiconductor particles has been shown to be an effective means of removing organic and inorganic pollutants from water. In this paper, the computer simulation of a distributive-type fixed-bed reactor that employs hollow glass tubes as light conductors was considered. The reactor configuration increases the surface-to-volume ratio while eliminating the possibility of light loss by absorption and scattering of the reaction medium. Immobilization of catalysts eliminated the need of any postprocessing filtration as required in a slurry reactor. The aim of the paper was to investigate the complex interplay of flow, diffusion, and chemical reaction on the degradation rate and to help achieve a better reactor design by computer simulation. In addition, a state-of-the-art computational technique, namely, distributive computing, was employed to expedite the speed of calculation and overcome the memory bottleneck present in a single workstation. The results show that the distributed computing technique is a very economical

and efficient method for overcoming difficulties, such as shortage of memory and long computation time, associated with computer simulations of reacting flows. A simple and powerful virtual supercomputer can be set up using the existing computer resources, such as a workstation farm, and reduces the dependency on single cabinet supercomputers.

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