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CFD MULTIPHASE MODELLING FOR EVALUATION OF GAS MIXING IN AN ANAEROBIC DIGESTER

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Abstract

Biogas production from municipal and industrial solid and liquid waste has captured the attention of engineers and managers both in the UK and globally due the substantial benefits for achieving environmental protection, energy generation and Green House Gas emission reductions. However, there are number of problems involved in scaling up experimental anaerobic digestion (AD) plants to field level plants. One such problem associated with AD is mixing, which is a vital component to segregate synthesized gas and biomass from digester liquid, to enhance homogeneity and to ensure adequate contact between bacteria and substrate in the AD. Such situations are well suited to Computational Fluid Dynamic (CFD) analysis, where models can be calibrated and validated using the pilot plant and can then be used to accurately simulate the performance of the large-scale reactors. The aim in this work has been to further understand and enhance the use of bubble mixing approaches to improve the performance of future bioreactors. A computational model has been developed to simulate the complex flows occurring in a digester. The paper discusses CFD simulations of a lab scale AD for evaluating mixing characteristics that provides understanding required for developing accurate simulations of mixing conditions in the large-scale systems with the reactor contents simulated for both Newtonian and non-Newtonian cases.

Key words

Green house gas (GHG), anaerobic digestion (AD), bubble mixing

Introduction

In recent years anaerobic digestion (AD) technology has been increasingly developed by environmental engineers and scientists to generate biogas and power from organic solid waste as a source of clean and green energy. AD technology not only generates biogas as an energy source, but also reduces the emissions of green house gases and has become a mandatory regulatory requirement for developed and developing countries in the management of solid wastes. This has resulted in the land-fill tax escalation scheme (LATS) implemented via the Renewable Energy Obligation Certificate (ROCs) in UK and in carbon offsetting and Certified Emission Ratings (CERs) in developing countries. The recent land fill allowances and tax escalation scheme (LATS) in the UK coupled with the ROC certificate require that 10% of UK's power demand must be generated through renewable energy by 2010 (Waste strategy, UK-2007). The Department of Environment, Food and Rural affairs (Defra, 2007), has estimated that the potential annual market for anaerobic digestion is \pm 400 million. In addition AD currently attracts two ROC's with a value of \pm 48/MWh (Shanmugam and Horan 2008).

Scum, foam, and froths are major causes of concern in anaerobic digesters as they have the potential to cause failure of the digester operation (inpart due to their prevention of gas release). Thus, the gas, liquid and solid (GLS) separation in an AD is vital for the success of the technology for any solid waste AD. Efficient mixing has been proved to increase the biogas production many fold enabling the recovery of further power from the solid waste. Bio-gas mixing has been reported to be less expensive and easier to operate than the impeller and slurry recirculated mixing (Cumiskey *et al*, 2003), but has not yet been optimised to maximise the biogas yield. In future reactor design, a high solid loading is necessary to reduce the size of reactor units, while maintaining a relatively low capital investment. High rate anaerobic digesters of high organic loading rates (OLR) and short hydraulic retention times have become an attractive co-digesting option for AD in recent years. However, high solid loading contributes to the problem of mixing inefficiency and more energy is required to complete the mixing. Lettinga (1981) suggested that minimal mixing may improve high solids anaerobic digestion by providing quiescent environmental conditions for bacteria.

The importance of mixing in achieving efficient substrate conversion has been reported by several researchers (McMahon et al., 2001; Stroot et al., 2001; Kim et al., 2002; Karim et al., 2005; Vavilin and Angelidaki, 2005; Vedrenne et al., 2007). The main factors affecting digester mixing are the mixing intensity and duration, the location of the feed inlet and outlet and and the type of mixing. However, the effect of mixing duration and intensity on the performance of anaerobic digesters are contradictory. For instance, adequate mixing has been shown to improve the distribution of substrates, enzymes and microorganism throughout the digester (Chapman, 1989; Lema et al., 1991), whereas inadequate mixing has been shown to result in stratification and formation of floating layer of solids (Stenstrom et al., 1983; Chen et al., 1990). In contrast continuous mixing was shown to improve biogas production compared with that of unmixed (Ho and Tan, 1985). The opposite results were also reported by several researchers (Ghaly and Ben-Hassan, 1989; Chen et al., 1990). However, the intermediate mixing appears to be the most optimal for substrate conversion (Smith et al., 1996; Dague et al., 1970). Minimal mixing was shown to be sufficient to distribute the feed adequately and stimulate the formation of new initiation centres (Vavilin and Zaikin, 1971) that are required for autocatalytic reactions (Field and Burger, 1985). At the other extreme, vigorous continuous mixing was shown to disrupt the structure of microbial flocks, which in turn disturbs the syntropic relationships between organisms thereby adversely affecting the reactor performance (Stroot et al., 2001; McMahon et al., 2001; Kim et al., 2002).. Furthermore, industrial reactors are often strongly inhomogeneous.

Bacterial sludges with a high solid loading are often characterised as non-Newtonian fluids i.e. the shear stress exerted on the sludge is not proportional to the induced shear rate. Mu *et al.,* (2007) stated that hydrogen producing sludges can possess highly non-Newtonian behaviour largely dependent on pH and extracellular polymeric substances associated with the sludge. Chen (1986) has concluded that livestock waste slurries and fermented liquor generally display non-Newtonian and pseudo plastic behaviour. It is evident from the

literature that anaerobic solid waste feedstock can show non-Newtonian shear thinning (pseudo plastic) behaviour.

Despite the importance of mixing in achieving efficient substrate conversion, there is no clear picture about the effects of mixing on the anaerobic digestion processes.

Computational fluid dynamics (CFD) has become a popular tool for reactor analysis, because it allows the investigation of local conditions in an arbitrary vessel size, geometry and operating conditions (Ranade, 2002). CFD techniques are being increasingly used for experiments to obtain the detailed flow fields for a wide range of fluid types. The capability of CFD tools to forecast the mixing behaviour in terms of mixing time, power consumption, flow pattern and velocity profiles is considered as a successful achievement of these methods and acceptable results have been obtained in many applications (Wu and Chen, 2007).

The literature review of numerical studies for unsteady gas-liquid flows identifies that bubble columns have been simulated using the Eulerian-Eulerian approach. In addition, it was observed that the Eulerian-Lagrangian approach could predict well the time-averaged properties (Delnoij *et al.*, 1997a, b, 1999; Lane *et al.*, 2002). This approach has the ability to account for the bubble size distribution in a simple manner which enables a more accurate description of the inter-phase forces, but at increased computational effort (drag, lift, virtual and other forces - Buwa *et al* 2002).

Anaerobic biohydrogen (bio-hydrogen) production from municipal and industrial solid waste research projects are currently being undertaken in the Pathogen Control Engineering Institute (PaCE) within School of Civil Engineering at the University of Leeds. As such, the geometry of one of their experimental reactor has been taken for this present study. As CFD modelling develops in this area it is anticipated that this experimental rig will allow a comprehensive validation of the CFD approaches. The three-dimensional anaerobic reactor tank being modelled represents a typical gas mixing lab reactor, which is used to generate hydrogen gas from municipal liquid and solid waste. The cylindrical geometry of the 3-D version of the tank was reproduced for the present study.

Overview of the study

In this work, CFD analysis has been undertaken in order to predict the mixing flow of a gas mixed anaerobic digester as a first step to optimize the process. This has been performed in two stages. Initially the reactor contents are assumed to behave as a Newtonian fluid (i.e. with constant uniform viscosity). This assumption is valid for the situation with low solid loading (up to 5%-Karim *et al.*, 2005). This allows for the mixing flow field induced by the gas injections to be investigated. A range of constant viscosity values based on experimental data from the anaerobic reactor are investigated.

In the later work a high solid content sludge that is used in the lab reactor to produce biohydrogen is investigated. In this case, experimental viscosity data has been measured for the sludge using rheometer. The reactor contents have been shown to behave as a shear thinning liquid following a power law relationship. A simulation has been undertaken to compare the difference in the mixing behaviour for the non-Newtonian liquid contents compared with that of a Newtonian fluid.

A brief review of a validated solution method which relates to the present work has been carried out and is presented in the following section.

A validated modelling method useful to this present study

The work of Buva et al., (2006) accurately predicts flow regimes induced through gas injections in a water filled bubble column. They have successfully implemented an Eularian-Lagrangian CFD approach that models the induced flow of a water bubble column, which has been validated with experimental data and numerical results. As such, elements of the work of Buwa et al (2006) have been reproduced by the authors for a two dimensional geometry to provide results which can be compared with the mixing flow of a continuous liquid phase reactor. Buwa et al., (2006) simulated the dispersed unsteady gas-liquid flow in a rectangular bubble column (0.2m width, 1.2m height, and 0.05m depth). They model the recirculatory flow generated by a locally/uniformly aerated sparger. The sparger has eight holes located at the centre of the bottom cross-section (holes of diameter 0.8mm, arranged in a square pitch of 6mm). The flow is considered as turbulent in the rectangular bubble column. The individual bubble's force balance is solved by pressure, buoyancy, gravity, lift and virtual mass forces. The plume oscillations of the Eularian-Lagrangian model with varied superficial gas velocities from 0.16 to 12.0 cm/s are carried out in the study. In this paper a superficial velocity of 0.19cm/s is taken for the same geometry and is modelled to provide a means to make an initial validation of the CFD approach. The results are in good agreement, with an oscillating plume generated (Figure 1) with a period of oscillation and induced flow path in good agreement with the result of Buwa et 2006 (the frequency of oscillation at a superficial velocity of 0.19m/s was found to be 10Hz.).

The process of accurately reproducing the CFD experimental work of Buwa for a specific geometry bubble column provided confidence that the same CFD approach will be appropriate to the new geometry, that of our anaerobic reactor.



Figure 1 Velocity field in the 2D rectangular narrow vessel showing the flow induced in a Newtonian fluid due to injected bubbles (superficial velocity 0.19cm/s)

Present study into the flow in the three dimensional reactor

Modelling the flow for a Newtonian fluid

A simplified case is taken where no flow in or out of the reactor is considered. This is a reasonable representation of the initial conditions in a real reactor at the start of a new process. The geometry of this model is defined to represent the geometry of the experimental lab reactor. A three-dimensional geometry of the cylindrical reactor tank was created (with diameter 115mm and height 300mm), as is shown in figure 2b. The simulation was carried using a mesh containing 53,170 hex/wedge volume elements created using a *Cooper* scheme.



Figure 2 (a) The laboratory scale anaerobic digester reactor modelled in this work, (b) 3D reactor mesh used in the CFD model

Fluent 6.3 was used as the CFD software for the model which offered several options for solution of a multi phase fluid. The following modelling approaches were taken:

- The contents of the reactor are initially considered as a continuous Newtonian fluid; in later stages a non-Newtonian model is implemented.
- A pressure based solver is used.
- The Reynolds Averaged Navier- Stokes equations are solved in this work.
- The flow in this reactor is considered as turbulent. Based on previous investigations the k- ε RNG (ReNormalization Group model) turbulence model was implemented in this work.

- The reactor contents are modelled as a liquid with a continuous single phase with the hydrogen being injected as a coupled Lagrangian discrete phase. The fluid density of the sludge is 1200 kg/m³.
- The hydrogen gas is injected at the centre of the bottom of the reactor from a 10mm diameter surface (cone shaped injection).
- Transient models are run to see how long it takes for the flow field to reach a steady-state condition.

Boundary conditions

The boundary conditions for the reactor are as follows: the bottom and the side walls are defined with non-slip conditions, the top of the fluid is in reality a free surface open to the air, in the simulation it is modelled as a wall with slip conditions (specified shear stress is zero). To account for bubble release it is defined to allow Lagrangian particles (injected hydrogen gas bubbles) to escape through it. In the experimental reactor this gas produced would be collected by an external tube in order for it to be reused for mixing purposes as well as being used for energy generation (converted into electricity). It is assumed that enough gas has been generated to provide continuous recirculation through the fluid for the purposes of mixing. In addition, the reactor produces gas during the ongoing anaerobic process that could additionally contribute to the mixing. This is not included in this model. All the simulations were performed on a dual processor Linux workstation with Intel PIV processors. In the transient simulations, the Eularian time step of 0.05s was used in all simulations.

Non-newtonian sludges

Anaerobic digester fluids are generally considered to be non-Newtonian (the sludge viscosity is a function of shear rate). Several authors have reported that most wastewater sludges are often characterised as pseudo plastic (shear thinning) fluids (Orf and Dentel 1992). This can be approximated in many cases by a power law equation:

$$\tau = \mathbf{k} \dot{\gamma}^{\mathrm{n}} \tag{1}$$

In equation 1.1 if n<1 it is a non-Newtonian shear thinning fluid and if n>1 it is a shear thickening fluid (if n=1, it is Newtonian).

The final stages of this study have been used to incorporate this complex non-Newtonian behaviour into the CFD model. Experimental viscosity data has been obtained from waste from leather fleshing combined with municipal solid waste as used in the experimental lab reactor. The measured relationship between apparent viscosity η and shear rate $\dot{\gamma}$ is shown in Figure 2 for this experimental data.





The experimental data fits a non-Newtonian power law relationship:

$$\eta = k\dot{\gamma}^{n-1} \tag{2}$$

The values for k and n are the average viscosity of the fluid (the consistency index) and the deviation of the fluid from Newtonian (the power-law index), respectively. The experimental work identifies values for k and n as 57.50 and -0.111, respectively. An upper and lower value for the viscosity have been used such that the maximum viscosity is 1Pa.s and minimum viscosity 0.005 Pa.s⁻

Computational model

The liquid-phase momentum conservation equation can be written as

$$\frac{\partial}{\partial t} (\rho_{1} \alpha_{1} U_{1i}) + \frac{\partial}{\partial t} (\rho_{1} \alpha_{1} U_{1i} U_{1j}) = -\alpha_{1} \frac{\partial P}{\partial x_{i}} + \frac{\partial}{\partial x_{j}} \left[\alpha_{1} \mu_{\text{eff}, l} \left(\frac{\partial U_{1i}}{\partial x_{j}} + \frac{\partial U_{1j}}{\partial x_{j}} \right) \right] - \frac{2}{3} \frac{\partial}{\partial x_{j}} \left[\alpha_{1} \mu_{\text{eff}, l} \frac{\partial U_{1m}}{\partial x_{m}} \right]$$

$$\alpha_{1} \rho_{1} g_{i} + M_{1i}$$
(3)

Where

 $ho_{
m l}$ is the liquid density

- α_1 , is the liquid volume fraction,
- U_1 is the mean liquid velocity,
- *P* is the pressure shared by both gas and liquid phases,
- $\mu_{
 m eff,1}$ is the effective viscosity of the liquid phase and

 M_1 accounts for the inter phase momentum transferred from all the gas bubbles to the liquid phase per unit time per unit volume.

The velocity of bubbles can be computed by solving the force balance over the individual bubbles:

$$m_{\rm B} \frac{du_{\rm Bi}}{dt} = F_{\rm Gi} + F_{\rm Di} + F_{\rm Li} + F_{\rm VM} + F_{\rm Pi}$$
(4)

Where m_B , is the bubble mass, u_B is the bubble velocity and F_G , F_D , F_L , F_{VM} , F_P are the forces due to the gravity, drag force, lift force, virtual mass force and pressure force, respectively. The bubble trajectories can be computed from the bubble velocities as:

$$\frac{\mathrm{d}x_{\mathrm{Bi}}}{\mathrm{d}t} = \mathbf{u}_{\mathrm{Bi}} \tag{5}$$

The forces due to pressure gradients, gravity and buoyancy as well as the drag forces exerted by the liquid on the bubble are incorporated in the model. Further information on the implemented discrete phase model are outlined in the Fluent user documentation.

The RNG k- \mathcal{E} Model

In this work the turbulence equations have been modelled using the RNG k- ε model. This model is derived from the instantaneous Navier-Stokes equations using (renormalization group) methods. This yields equations for k and ε .

$$\frac{\partial(\rho k)}{\partial t} + \nabla .(\rho k u) = \nabla .(\alpha_k \mu_{eff} \nabla k) + G_k + G_b - \rho \varepsilon - Y_M + S_k$$
(6)

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla \cdot \left(\alpha_{\varepsilon}\mu_{\text{eff}}\nabla\varepsilon\right) + C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_{k} + C_{3\varepsilon}G_{b}\right) - C_{2\varepsilon}\rho\frac{\varepsilon^{2}}{k} - R_{\varepsilon} + S_{\varepsilon}$$
(7)

The R_{ε} term in the equation 1.7 is the main difference between the RNG and standard k- ε models. The RNG model equations and the other equations presented above were solved using Fluent 6.3. The spatial terms were discretized using standard first order schemes.

Results and discussions

Transient case for the Newtonian fluid

The gas injections are modelled as coupled Lagrangian particles injected over a circular (diameter 10mm) area. Fifty separated streams are used in each case and the total mass flow rate of the hydrogen bubble is 9.4×10^{-06} kg/s (or 0.1 cm³/s).

Results from the Newtonian model are shown in figure 4 (a)-(f). These show the instantaneous flow field developing for the transient simulation following initiation of the bubbles being injected. The flow fields are plotted on a plane passing through the centre of the vessel. Due to the symmetry of the reactor, the flow is axi-symmetic throughout the vessel, it is reasonable to consider that that the flow on this plane is representative of the whole reactor. As would be expected there is a high velocity zone entering through the injected point and moving vertically up to the centre of the vessel.

The developing flow field obtained from the transient simulation allows for the initiation of mixing to be observed (figures 4 (a) –(f)). Instantaneous time steps are shown for 1 second, 2, 3, up to 10 seconds. At 10 seconds the flow has reached steady-state conditions. Although a state very close to steady is achieved after approximately 3 to 4 seconds. Flow in upper section of the reactor is above 0.05m/s which is adequate for mixing the contents of a reactor in this region for a reactor of this size. The flow in the lower region is below 0.05m/s and much of it is significantly below this value indicating that there will be relatively poor mixing in this region.





Figure 4 Simulated mixing behaviour of a Newtonian liquid sludge inside the 3D reactor following the start of hydrogen gas injections into the vessel: (a) to (f) show flow coloured by velocity at t=1, 2, 3, 4, 8, 10 seconds, respectively

Newtonian fluid: constant viscosities of 0.001, 0.01, 0.1, and 1 Pa.s

The path lines provide information on the mixing region (the areas of optimum mixing) and dead zones (i.e where extremely low level mixing occurs) within the reactor. In figures 5 (a)-(c) the steady-state flow fields for fluids with increasing uniform viscosities of 0.001, 0.1 and 1 Pa.s, are shown respectively.

In the first simulation with a viscosity of 0.001Pa.s is taken which is equivalent to that of water at room temperature.. In this case away from the central jet, the velocity is higher nearer to the top of the reactor. It can be observed that there are recirculation regions near the top corners and very low mixing at the bottom of the reactor (figure 2.2(a)). The peak velocity in the reactor, as would be anticipated, is in flow of the central jet where the velocity magnitude is above 0.4 m/s.

Figure 5 (b) shows the steady-state flow field for a viscosity of 0.01Pa.s. It can be observed that there is one primary recirculation zone with its centre close to the top of the reactor and a secondary recirculation zone at the bottom of the reactor. There is also a high velocity region at the centre of the reactor. Velocities are mostly above 0.03m/s in the upper primary recirculation region where mixing is shown to be good. Velocities below 0.01 m/s are visible in the small stagnation zones and at the corners points of the recirculation zones. Relatively low flow rates are also present in the lower region of the reactor. The secondary recirculation zones in the lower region have significantly lower velocities of below 0.0025 m/s in which mixing is poor.

As can be seen in Figure 5 (c), for the case with a velocity of 0.1Pa.s, there is no secondary recirculation zones in the reactor. High velocities of 0.2 m/s are present in the centre of the vessel with recirculation on both sides. These recirculations are present only in the top of the reactor with much lower velocities lower down. The mixing in the upper region is reasonable, but with lower velocities when compared to a similar region in the lower viscosity cases. The mixing in the lower region is again very poor.





The flow field for the case of a constant viscosity of 1 Pa.s is shown in Figure 6. For this high viscosity case there is only one major recirculation zone, The velocity of the flow is significantly reduced when compared with the lower viscosity models. The flow in the region close to the centre bubble channel is still relatively high at above 0.01m/s, but in the rest of the reactor there are very low flow velocities and as such it will have significantly reduced mixing.





Non-Newtonian viscosity simulations

A transient simulation has been undertaken for the non-Newtonian viscosity model of the fluid. The experimental data obtained from the rheogram is shown in the figure 2. The power law model provides reasonable agreement with the viscosity over wide range of strain rates. As such, the power law model has been implemented in the region of 0.001 Pa.s to 1 Pa.s. These values are implemented as the high and low limits. The flow fields are shown for a non-Newtonian transient simulation in figures 7 (a) to (g).





Comparison with the Newtonian case:

In the transient simulations it takes a similar time for both the Newtonian and non-Newtonian cases to reach a fully steady-state solution, however the Newtonian (viscosity =0.001 Pa.s) case gives a flow field that is approximately steady state after only 3 seconds. It takes around 6 seconds in the case of the non-Newtonian case. In the steady-state case (figure 7 (g)) it is possible to observe a single recirculation zone with velocities above 0.02m/s in a large proportion of the reactor. However, there are much lower velocities at the corners. Although the velocities are generally lower in the non-Newtonian case when compared to the Newtonian ones, it appears that the region of mixing is larger. This is an interesting result as it appears to indicate that there could be more homogenous mixing in the non-Newtonian case. However, more work needs to be undertaken in this area to investigate a range of gas flow rates in addition to verification and validation of the Non-Newtonian approach before any general conclusions can be drawn.

These result clearly show that the flow induced for a shear thinning liquid appear to give notable differences to the Newtonian cases. Further work is needed (including full experimental validation of these results), but they provide a useful basic implementation of the power law model in non-Newtonian fluid behaviour case

Conclusions

The three-dimensional mixing flow induced through injected hydrogen bubbles (in order to simulate gas recirculated mixing) has been undertaken for a pilot scale anaerobic reactor. The CFD simulations have been performed for a range of constant viscosities in addition to the implementation of a power-law viscosity model that accounts for the experimentally measured non-Newtonian behaviour of a particular anaerobic sludge that is currently being investigated at the University of Leeds. Transient CFD simulations are performed in order to observe the progression of flow over time following the start of the bubble injections. In the experimental facility the bubble mixing is often performed as relatively short bursts and as such the time taken to reach steady flow is of interest.

A summary of the research outcomes include:

- In the case of the transient simulations for the range of liquid sludges with different constant viscosities (with each case the flow rate of hydrogen through the reactor was kept at 9.4 x 10⁻⁶ kg/s in line with those used in an experimental set up at the University of Leeds), the predicted velocity flow fields allow the effect of increasing viscosities to be observed. It is apparent that when fluid viscosity approaches 1Pa.s the mixing in the reactor is very low.
- The mixing induced in the case of viscosities in the range 0.001 Pa.s to 0.01 Pa.s appear to give reasonable mixing in large areas of the vessel. However, in the cases with increased viscosity (above 0.1Pa.s) the mixing degrades with significant increases in dead zones.
- In the transient case study for a viscosity of 0.001Pa.s it was observed that the reactor takes between 6-7 seconds of real time to reach a steady-state condition (although the flow field is approximately steady state after only 3 seconds).
- For the case where a non-Newtonian power law is implemented in the CFD model (based on the experimental data from real digester sludge) the flow takes slightly longer than the Newtonian case to reach steady flow (around 9-10 seconds). In this case the mixing appears more homogeneous when compared to Newtonian fluid velocity of 0.001Pa.S.

Future work to improve and validate the model predictions

Further mesh refinement will be undertaken to capture specific flow features to attempt to improve the accuracy of results and to reduce model computational times (e.g. in a areas with high flow rates and large shear rates).

Further refinement and investigation of CFD techniques is necessary. This includes further development of the two-phase modelling and verification of the turbulence model interaction with the viscosity model.

Experimental validation will be conducted for both Newtonian and non-Newtonian simulations using a transparent bubble mixed reactor using both dye tracers and ultrasonic equipment.

Further development and validation of sparger modelling and design will be undertaken.

An investigation on the impact of scaling up the reactor geometry to a full production capability anaerobic digester will be undertaken in the next phase of work.

Based on the results of this and future work it will be possible to implement changes to the design of reactor geometry (e.g. inclusion of Baffles) for Newtonian and non-Newtonian fluids in order to design optimum mixing conditions.

An investigation into optimum flow rates for a range of different sludge rheology will be undertaken.

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