Essential Readings in Light Metals: Alumina and Bauxite.
Edited by Don Donaldson and Benny E. Raahauge.

ALUMINA CRYSTALLISER MIXING USING CFD

Jean Perron and Jacques Larocque
Alcan International Limited,
Arvida Research and Development Centre
P.O. Box 1250, Jonquière (Québec)
CANADA, G7S 4K8

ABSTRACT

Within Alcan, some plants are presently converting part of their batch precipitation circuit to a continuous mode. This paper presents how commercial Computational Fluid Dynamics (CFD) software can be used to optimise the retrofit by examining the homogeneity of mixing in various tank configurations and mixing systems.

INTRODUCTION

The following illustrates how hydrodynamic modelling through Computational Fluid Dynamics (CFD) may be used in the context of the Bayer process for the extraction of alumina trihydrate from bauxite. The case study discussed here is in the crystallisation area where high alumina concentration liquor is mixed with seeds to accelerate the decomposition of alumina in solution to solid alumina trihydrate for the production of metallurgical grade alumina.

Introduction to the Process Problems

Several of Alcan's older plants are still using the batch precipitation technique. An effort is being made to convert these plants to some form of continuous precipitation in as for as the economics justifies it. Some of the plants are converting a number of batch tanks to serve as continuous precipitators in the front end of the circuit; the justifications to do so are numerous; namely to stabilize seed charges by going from batch to continuous seeding, to minimize manpower for the same reason, to lower residual soda by lowering the initial supersaturation, to facilitate the use of cooling systems to control the cooling profile in precipitation, etc... Plants are then converting part of the circuit preferably the front portion, to a continuous mode, the back end staying in a batch mode where the feed is a premixed slurry of liquor and seeds in which precipitation has already begun. Most often it appears uneconomical to convert a complete batch plant to a continuous mode if the plant was not constructed for this in the first place.

At most plants, it is more economical to convert actual batch tanks to continuous precipitation by some retrofit rather than building new tankages; another component of the problem when retrofitting is to assure adequate mixing within the tank; this is important:

1) to avoid by-passing high ratio liquor;
2) to assure adequate homogeneity of solids (seeds);
3) to assure homogeneous concentration of alumina in solution, in order to obtain a minimum supersaturation, hence minimum residual soda.

In order to attain objectives explained in the previous paragraph, it was decided to build a hydrodynamic model to evaluate different design alternatives instead of resorting to expensive experimental modifications of full-size tank. Such a model can give hydrodynamic patterns that, if not accurate in absolute term, can discriminate easily between different alternatives compared to some base case.

Description of the Physical Tank

The precipitator to be modelled is a 900 m^3 tank with a cone bottom; the pregnant liquor enters from the top as does the seed. The tank is maintained full and the outlet can be placed at different levels in the tank. A recirculation line provides agitation by running from bottom of the cone to a tangential re-entry at the top. This is illustrated in Figure 1.

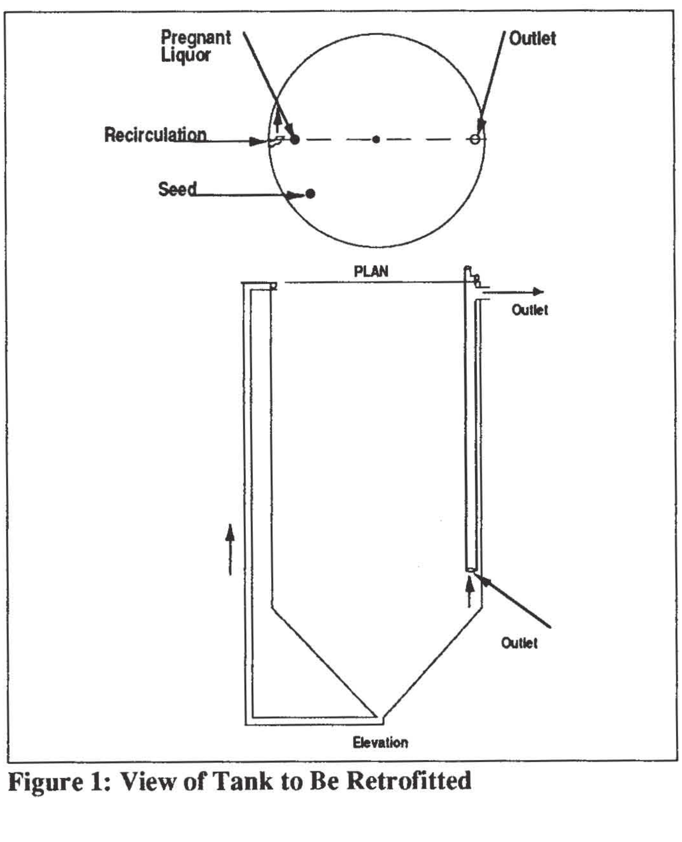

Figure 1: View of Tank to Be Retrofitted

Description of the Mathematical Model

Because the physical problem has no symetry in any direction, a three-dimensional (3-D) model was constructed; also because the tank is a cylinder, cylindrical coordinates (r,θ,z) were used. The problem was assumed and solved for steady state according to standard continuity equation which can be found in all usual textbooks [1,2].

The solution of the transport equations is performed by PHOENICS [3] software wich uses the finite volume method. The geometry is at the actual scale of the precipitator. The network consists of 3312 finite volumes in which all the variables are calculated as illustrated in Figure 2; the grid is finer at the top and bottom of the tank to account for greater changes in velocity fields. The upper liquid surface is considered a free surface. The equations are solved not only for conservation and momentum of the liquid but also the solid phase. Although the PHOENICS software can deal with 10 class fractions of solid only 3 were used to limit computing time; the so-called algebraic slip model is used to incorporate solids. The precipitation reaction is also included in the model, to evaluate the concentration of dissolved alumina in all parts of the tank as the reaction proceeds from dissolved alumina to solid alumina trihydrate.

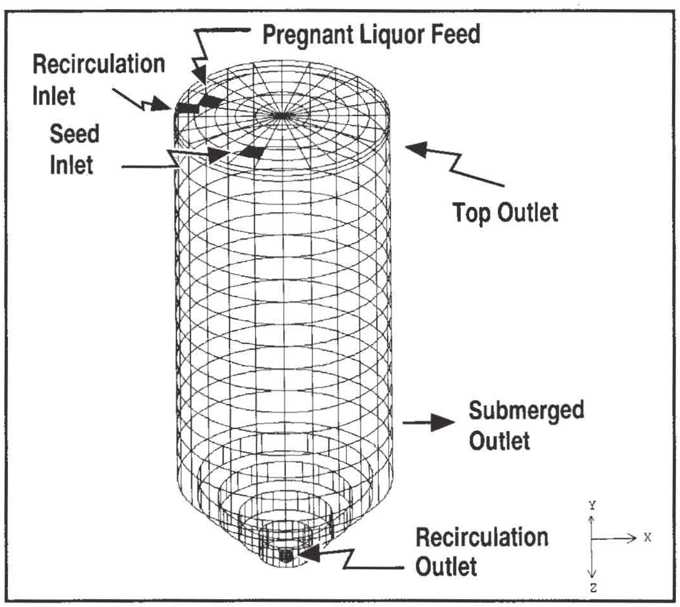

Figure 2: Grid Configuration

The calculated variables are:

p : pressure

u_θ, v_r, w_z : angular, radial and axial velocities

k, ε : turbulent kinetic energy and its dissipation rate (k - ε model)

m_1, m_2, m_3: mass fraction of 55 μm, 75 μm and 95 μm particles

ρ_m : liquid/solid mixture density from:

$$\frac{1}{\rho_m} = \frac{1-\Sigma m_i}{\rho_l} + \Sigma \frac{m_1}{\rho_i}$$

where:

ρ : density

m : mass fraction

i : solid fraction subscript

l : liquid subscript

m : mixture subscript

μ_m : liquid/solid mixture viscosity from:

$$\mu_m = \mu_l \left(\frac{1 + .5\Sigma m_i}{(1 - \Sigma m_i)^4} \right)$$

C : dissolved alumina concentration (at r, θ, z) from:

$$\frac{dC}{dt} = k\,(C - C_{eq})^2$$

where:

t : time

k : kinetic constant (including surface area)

C_{eq} : equilibrium alumina concentration

Initial and Boundary Conditions

Initial conditions are as follows:

- Pregnant liquor at the entry contains 127 g/L of alumina at a flow of 220 m³/h.
- Seed is injected at a flow rate of 70 m³/h. To produce a concentration of 195 g/L after mixture with the pregnant liquor.
- Initially the tank is assumed to be full of pregnant liquor at 195 g/L of solids.

Boundary conditions are the following:

- There is a no flow condition at the wall of the tank.
- At the top of the tank, there is a free surface.

RESULTS

Results Presentation

Essentially the results are contained in a huge file where we have for all the 3312 volume elements results of all the calculated variables (≃ 15). For interpretation, results have to be compiled either in picture form with iso-contour or in statistical format for all the calculated volumes. Both forms are presented in this study.

Several cases were tried during the course of the work but only a few will be shown here.

The 3-D model calculates the liquor velocities, as well as the dissolved alumina concentration Al_2O_3 (d) in the precipitator. For each case studied a Fortran program coupled with PHOENICS permits the calculation of:

- the average dissolved alumina concentration Al_2O_3 (d) in the precipitator;
- the concentration of Al_2O_3 (d) at the outlet;
- the quantity of Al_2O_3 (d) precipitated;
- the standard deviation of the concentration in the reservoir;
- the volume percentage of the reservoir where the Al_2O_3 concentration is ± 2 g/L of that at the outlet.

The results are compared in the following tables. Two series of simulations carried out in order to study the effect of recirculation flow and the effect of the overflow location.

A criteria for the degree of mixing was chosen; all 3312 are scanned after the model has achieved convergence and a minimum of 80% of those are required to be at ± 2 g/L of the outlet dissolved alumina; this assures that not only the concentration in the reservoir is homogeneous but also there is no by-passing of the liquor. Another way of looking at the results is to look at the standard deviation of the results of dissolved alumina.

Effect of Recirculation Flow on the Concentration in the Precipitator

The model outputs are shown in Table I for the effect of increasing recirculation flow. Figures 3 to 5 are illustrating the first three cases in which the recirculation flow is taken from 150 m³/h to 1000 m³/h. Figures 3a), 4a), and 5a) represent a cut view of the tank while Figures 3b), 4b), and 5b) represent a top view of the tank with isoconcentration lines.

Table I – Effect of Recirculation with the Overflow at the Top of the Reservoir

Case #	Recirculation Flow (m³/h)	Alumina Précipitated (g/L)	$(Al_2O_3)_d$ Average in the Reservoir (g/L)	$(Al_2O_3)_d$ Reservoir Exit (g/L)	% Volume ± 2 g/L at the Exit and S. Dev.	Comments
1	150 Overflow Opposite	35.1	95.9 Figure 3a)	91.9	27.3% 5.8 g/L	Not Short Circuit Figure 3b)
2	300 Overflow Opposite	30.6	94.0 Figure 4a)	96.4	36.7% 5.8 g/L	Weak Short Circuit Figure 4b)
3	1000 Overflow Opposite	30.7	91.8 Figure 5a)	96.3	1.7% 1.6 g/L	Strong Short Circuit Figure 5b)

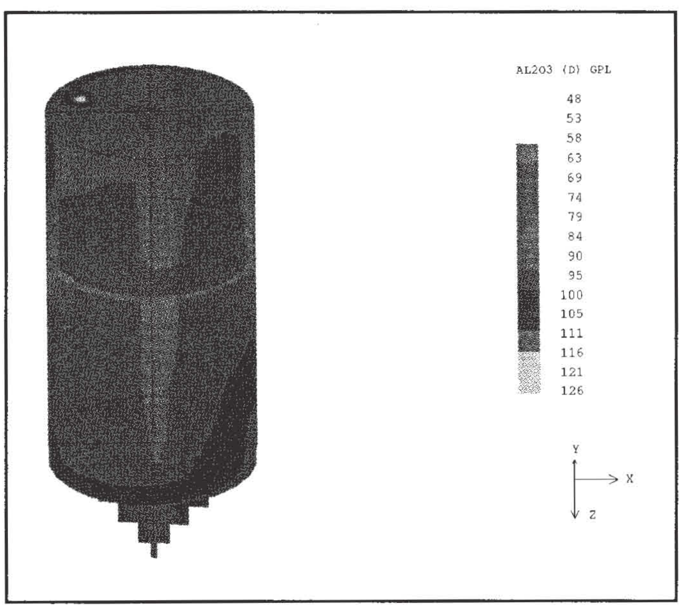

Figure 3a): 150 m³/h Recirculation with Top Outlet

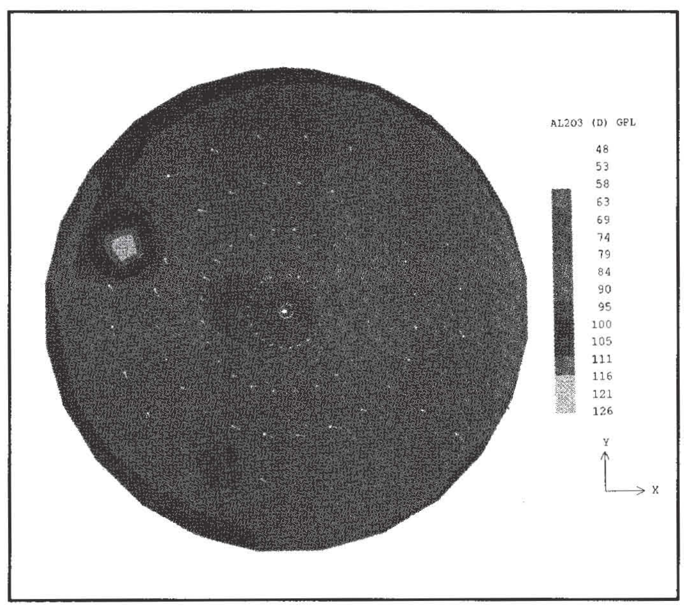

Figure 3b): 150 m³/h Recirculation with Top Outlet

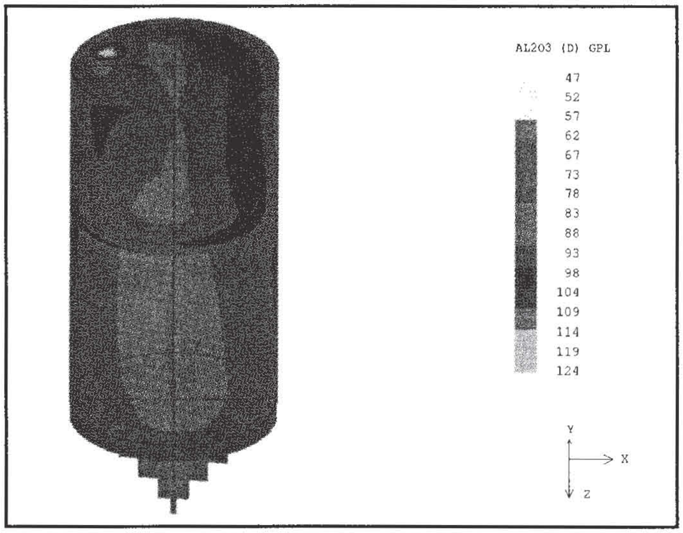

Figure 4a): 300 m³/h Recirculation with Top Outlet

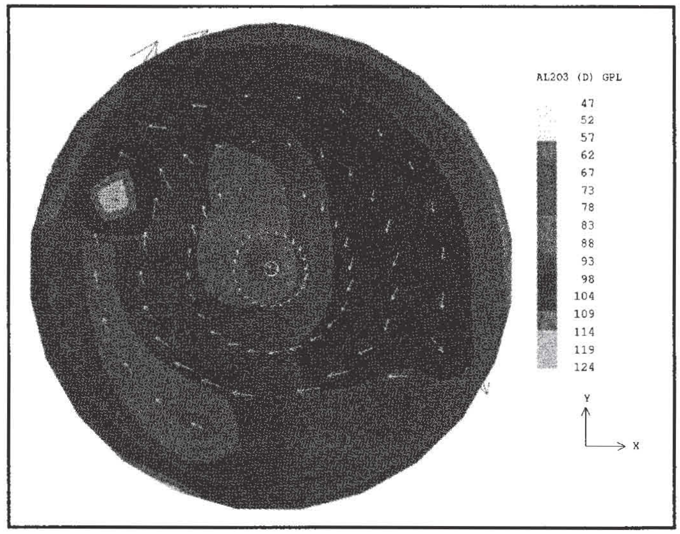

Figure 4b): 300 m³/h Recirculation with Top Outlet

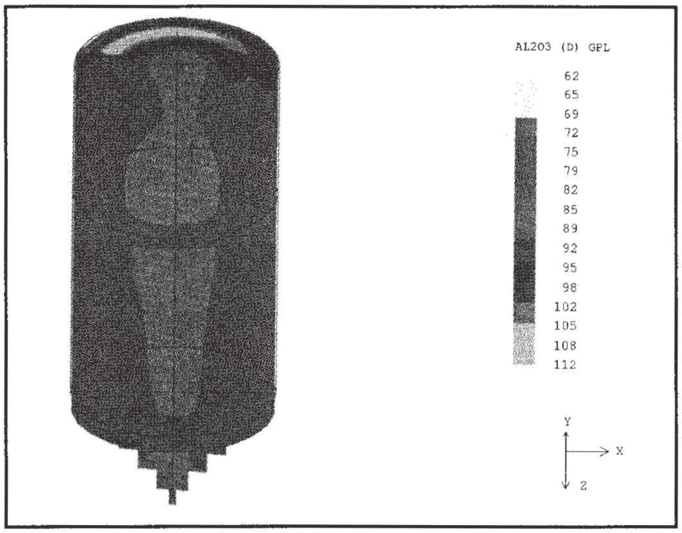

Figure 5a): 1000 m³/h Recirculation with Top Outlet

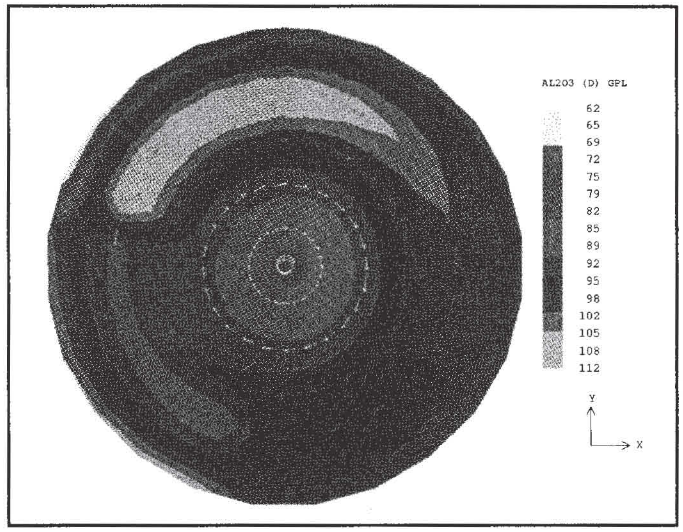

Figure 5b): 1000 m³/h Recirculation with Top Outlet

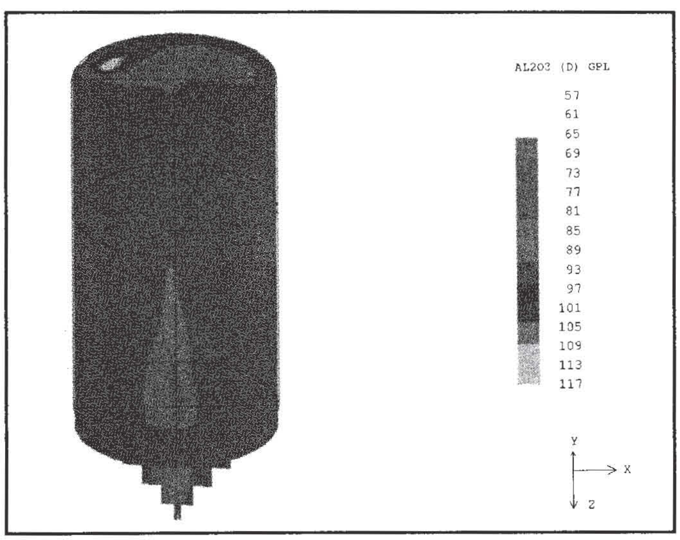

Figure 6a): Cut View with Outlet 2/3 Down the Tank at 1000 m³/h Recirculation

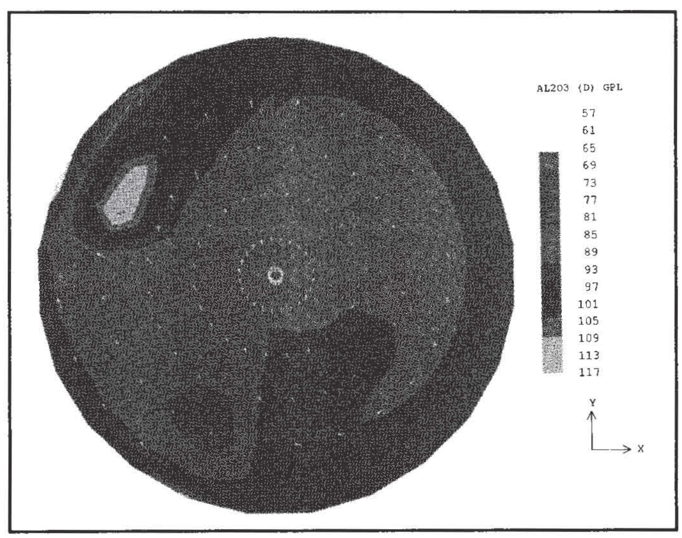

Figure 6b: Top View with Outlet 2/3 Down the tank at 1000 m³/h Recirculation

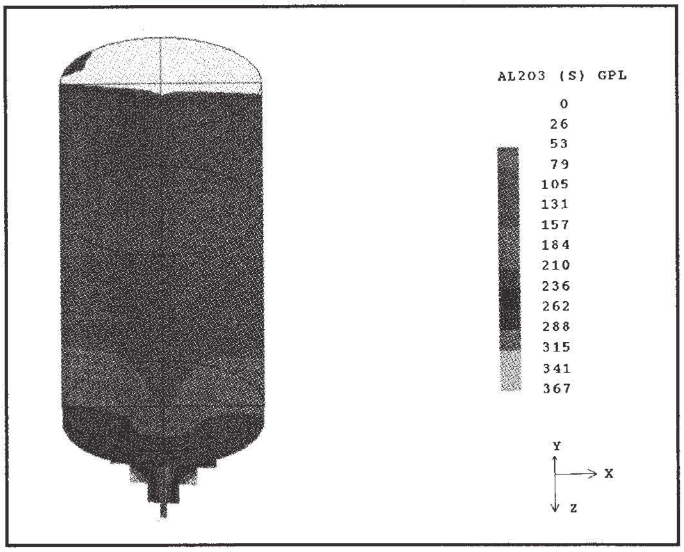

Figure 7: Solids Profile with Outlet 2/3 Down the Tank at 300 m³/h Recirculation

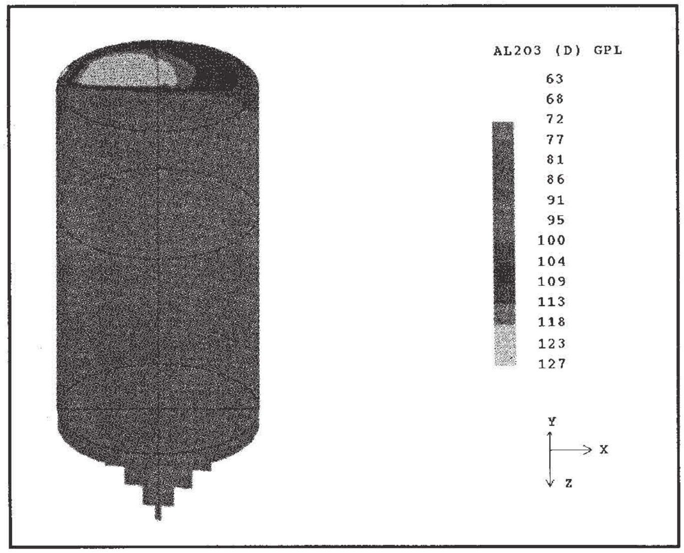

Figure 8: Dissolved Alumine Profile with Outlet 2/3 Down the Tank at 300 m³/h Recirculation

We can observe that, as the recirculation increases there is a direct short circuiting of the pregnant liquor to the overflow caused by the entrainment of pregnant liquor to the outlet by the recirculation flow. In addition, at a recirculation rate of 150 m^3/h the percentage of the reservoir, volume within ± 2 g/L of the outlet value is low at 27.3%. The acceptable target is of the order of 80%. For these reasons, it was concluded that the position of the outlet should be changed in order to avoid the short circuiting of the pregnant liquor. To remedy the short-circuiting situation, it was considered necessary to locate the overflow as far as possible from the liquor entry. Another observation can also be drawn from Table I; Case I gives the highest productivity and is the only one in which the average dissolved alumina in the reservoir is higher than the outlet; this is due to the plug flow nature of the flow pattern: a channel is formed that goes from the liquor inlet to the lower part of the tank and back up to the outlet. Although this is good for productivity, it is undesirable from a good mixing point of view.

<u>The effect of the Overflow Location on the Concentration in the Precipitator</u>

The location chosen was diametrically opposite the entry of the pregnant liquor, immersed to a point 2/3 of the distance down from the liquor surface of the reservoir. the results obtained are shown in Table II. From that Table we can see that for cases 5 to 7, the % volume at±2 g/L is significantly improved going from a maximum of 37% for top outlet to 89% for the submerged outlet.

Table II – Effect of the Overflow Location with Different Recirculation Flows

Case #	Recirculation Flow (m³/h)	Alumina Précipitated (g/L)	$(Al_2O_3)_d$ Average in the Reservoir (g/L)	$(Al_2O_3)_d$ From the Reservoir (g/L)	% Volume ± 2 g/L of the Overflow and S. Dev.	Short Circuiting of Liquor to the Overflow
5	300 Overflow Opposite Submerged	32.0	94.6	95.0	55.1% 6.5 g/L	None
6	675 Overflow Opposite Submerged	32.7	93.4	94.3	74.9% 4.8 g/L	None
7	1000 Overflow Opposite Submerged	33.4	93.0 Figure 6a)	93.6	88.6% 3.3 g/L	None Figure 6b)

It can be seen that the submerged overflow is a good arrangement which avoids short circuiting of the pregnant liquor, even when the recirculating flow is high as shown in Figure 6b) compared to 5b. It should be noted that, in order to attain the target, of 80% or more of the volume of the reservoir at ± 2 g/L of the overflow concentration, the recirculating flow must be over 800 m^3/h (from interpolation).

Results with Solids

As a first step in the solution of the problem, solids were assumed to be homogeneous in the tank and the fluid is considered as one phase. The solids are added in a second step as a set of 3 different monosize fractions as stated above to simulate the size distribution. The algebraic slip model of PHOENICS was used for the solids.

A FORTRAN program calculates for each case the solid variables:

- the average concentration of Al_2O_3 (s) in the precipitator;
- the concentration of Al_2O_3 (s) in the overflow;
- the standard deviation of the solid concentration in the reservoir;
- the percentage of the reservoir volume where the concentration of Al_2O_3 (s) is within ± 50 g/L of that in the overflow.

The results are compiled in Tables III and IV. The computing time is much longer due to the presence of the solids; these add as many variables as there are mass fractions. In the present case, there are three independent fractions together with three associated Reynolds numbers. With the density and viscosity, there are eight additional variables to calculate for each finite volume.

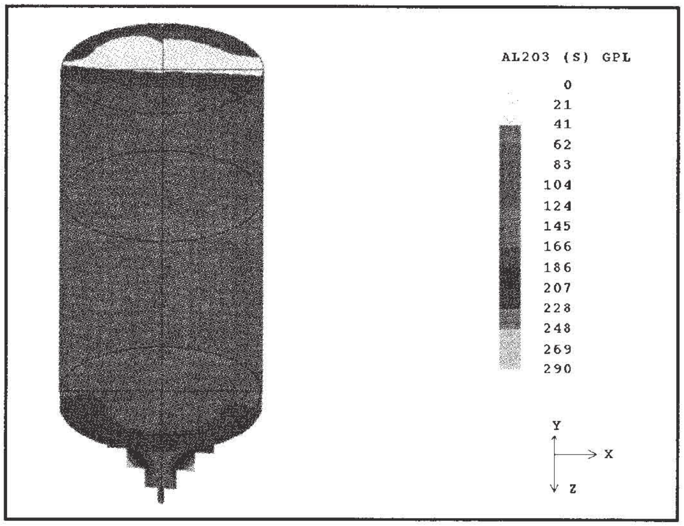

Figure 9: Solids Profile with Outlet 2/3 Down the Tank at 1000 m^3/h Recirculation

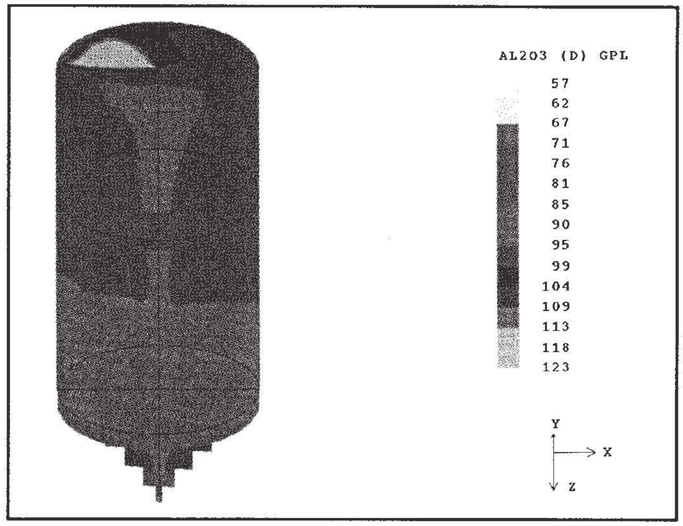

Figure 10: Dissolved Alumina Profile with Outlet 2/3 Down the Tank at 1000 m^3/h Recirculation

Table III– Solids Concentration Results

Case #	Recirculation Flow (m^3/hr)	$(Al_2O_3)_s$ Average in the Reservoir (g/L)	$(Al_2O_3)_s$ Reservoir Outlet (g/L)	% Volume ± 50 g/L Solid of the Outlet and Std. Dev.	Short Circuit of Liquor to the Outlet
9	300 Submerged Outlet 2/3	184.7 Figure 7	189.1	83% 57.5 g/L	None
10	1000 Submerged Outlet 2/3	174.0 Figure 9	182.8	95.8% 31.1 g/L	None

Table IV– Dissolved Alumina Concentration Results

Case #	Recirculation Flow (m^3/hr)	Alumina Precipitated (g/L)	$(Al_2O_3)_d$ Average in the Reservoir (g/L)	$(Al_2O_3)_d$ Outlet from Reservoir (g/L)	% Volume ± 2 g/L of the Overflow and Std. Dev.	Liquor Short Circuit to the Overflow
9	300 Submerged Outlet 2/3	33.5	96.3 Figure 8	93.5	41.6% 3.2 g/L	None
10	1000 Submerged Outlet 2/3	33.1	95.2 Figure 10	93.9	90.8% 2.0 g/L	None

Effect of Overflow Location and the Recirculation Flow on the Concentrations of Solids and Dissolved Alumina in the Precipitator

In Table III, it may be seen that increasing the recirculation flow improves the homogeneity of the total solids in the precipitator. As a matter of fact, the standard deviation of the solids concentration was reduced by 26.4 g/L, a reduction of 46%, when the recirculation rate was increased from 300 to 1000 m^3/h. For this reason, it is clearly advantageous to increase the recirculation flow to the higher value i.e. close to 1000 m^3/h.

In Table IV, the results of the alumina precipitation model are shown. One may see that, as the recirculation flow increases, the standard deviation of the dissolved alumina decreases, this is in agreement with the results already presented in the first part of this study. As a matter of fact, cases 9 and 10 are similar to cases 5 and 7, except that they include the effects of solids on hydrodynamic behavior mainly through variable density and viscosity. One can see a certain similarity between the simulations with and without solids; this shows that it was acceptable to ignore the solids in the first study, and the results of that study remain valid.

Figures 7 to 10 show respectively the profile and the solids concentration and the dissolved alumina for the two recirculation flows.

We are presently coupling completely the solids and the precipitation reaction to take into account the variation of seed surface area in one and all finite volumes of the grid. Although not very important in this case because the tank is rather well mixed, it is important to do so in poor homogeneity precipitation where segregation can be important.

GENERAL CONCLUSION

The PHOENICS sofware has proven to be a useful development tool for this type of project. However, as the problem gains in complexity (solids addition, strong turbulence, small grid network, etc.), convergence becomes difficult and computational time can increase dramatically. The more complex simulations done in this study have required up to 8 hours on a HP-730 workstation; this implies that a balance must be struck between complexity and results.

Validation of results through experimental work is an issue that has not been fully addressed although we in Alcan have been able to simulate phenomena that we are identifying in our reactor/precipitator e.g. ratholing of tanks, high solids in low velocity area, tank outlet concentration and solids in dynamic hydrodynamic modelling. We recommend as in most modelling or simulation, to work from a base case with relative results instead of absolute results because they involve much more knowledge.

REFERENCES

[1] Convective Heat and Mass Transfer, Kays and Crawford, McGraw-Hill, 2 Ed., 1980.

[2] Transport Phenomena, Bird, Stewart and Lightfoot, Wiley, 1960.

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