

VisiMix Forum

May 17, 2017

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Retiree from The Dow Chemical Company



VisiMix Forum

- ***Community of expert VisiMix users***
- ***Understand process results and mixing parameters***
- ***Future Forum presenters - expert VisiMix users***
 - ✓ ***Address proven protocols and techniques for effective process r&d, scale up, and production***
 - ✓ ***Case studies of different unit processes in the chemical process and allied***

Industrial Mixing Expert

The surest way to be an expert in something is to have the passion to

Learn
Apply
Document
Teach

Resources



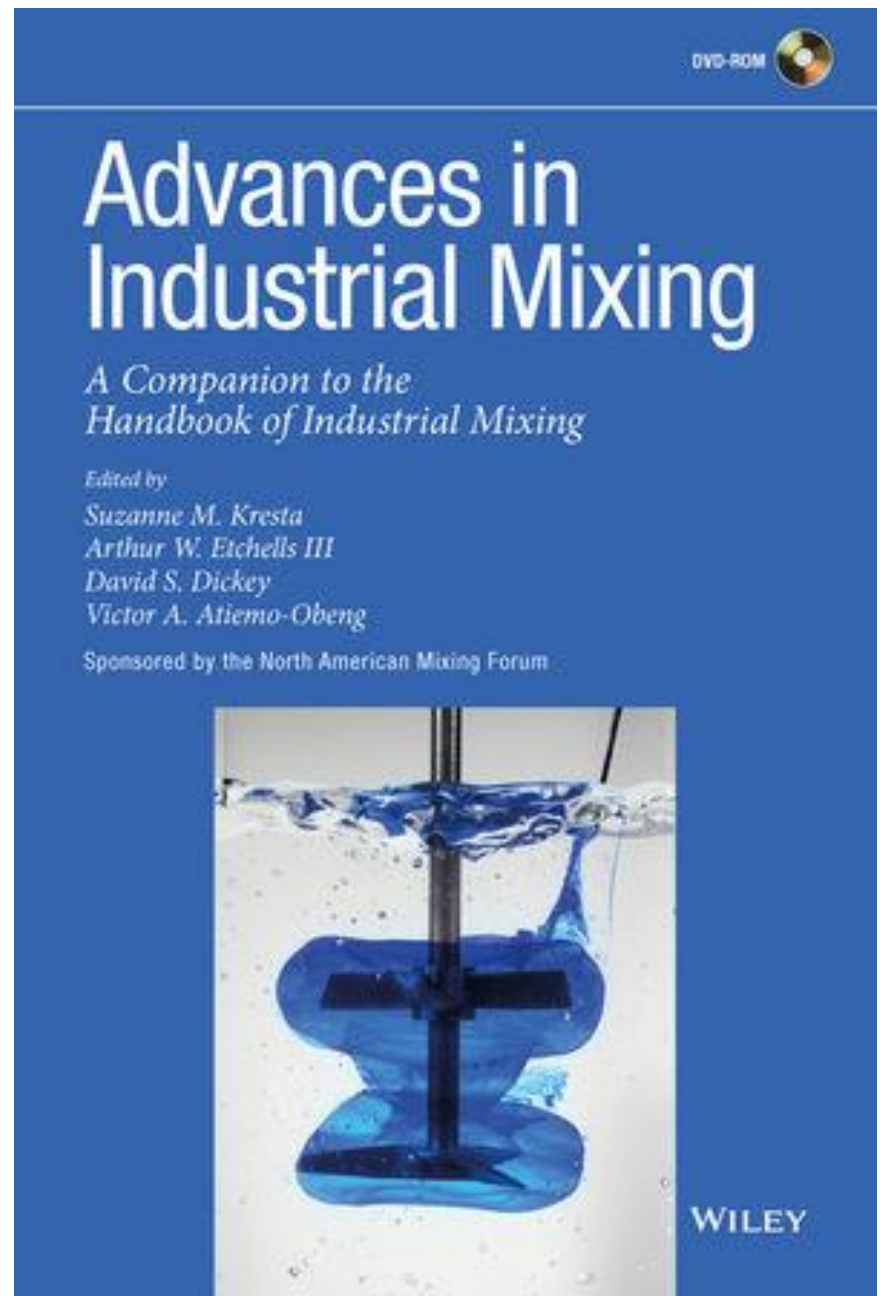
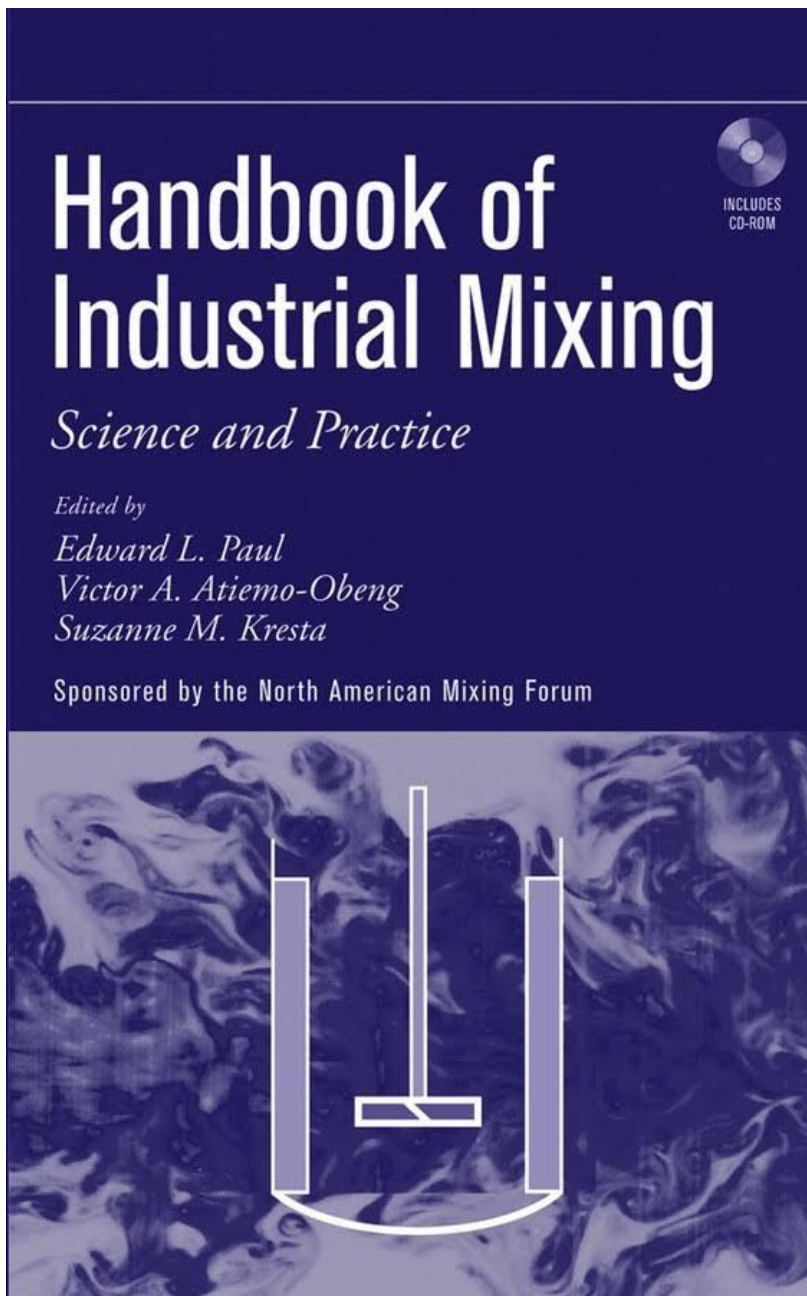
North American
Mixing Forum

<http://www.mixing.net>



Fluid Mixing Processes (FMP)
An Industrial Consortium

Resources



Resources



VisiMix Turbulent

Low viscosity liquids and multi-phase system



VisiMix DI

Combined mixing devices



VisiMix Laminar

Highly viscous and non-Newtonian



VisiMix RSDE

Rotor Stator Disperser and/or Emulsifier



VisiMix Pipeline

Carreau rheological model



VisiXcel

Creating an organized data base

VisiMix

“It is a **highly accessible PC software** for mixing calculations available from VisiMix Ltd., an Israeli company. It is **a rating calculation tool** for both non-reactive and reactive mixing involving blending, solid suspension, gas dispersion, liquid-liquid dispersion, or heat transfer processes in stirred vessels. It calculates the important process parameters for single- and two-phase systems – power consumption, circulation rates, local concentrations of solutes and suspended particles, drop size, concentrations of reactants, etc ...”



***VISI MIX – PRODUCTIVITY TOOL FOR
THE ANALYSIS, SCALE-UP AND
DESIGN OF MIXING PROCESSES IN
STIRRED TANKS***

Victor Atiemo-Obeng, Hua Bai, Richard Cope, The Dow Chemical Company
Cesar Gonzalez, Styron LLC

VisiMix International Conference
Boston, MA
July 13-15th 2011

VisiMix



VisiMix Turbulent

Low viscosity liquids and multi-phase system



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Highly viscous and non-Newtonian



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MIXING ASPECTS COVERED:

Hydrodynamics

Single phase Mixing (Blending & Reaction)

Batch, Semi-Batch, Continuous

Liquid-Solid mixing

Liquid-liquid mixing (liquid dispersion)

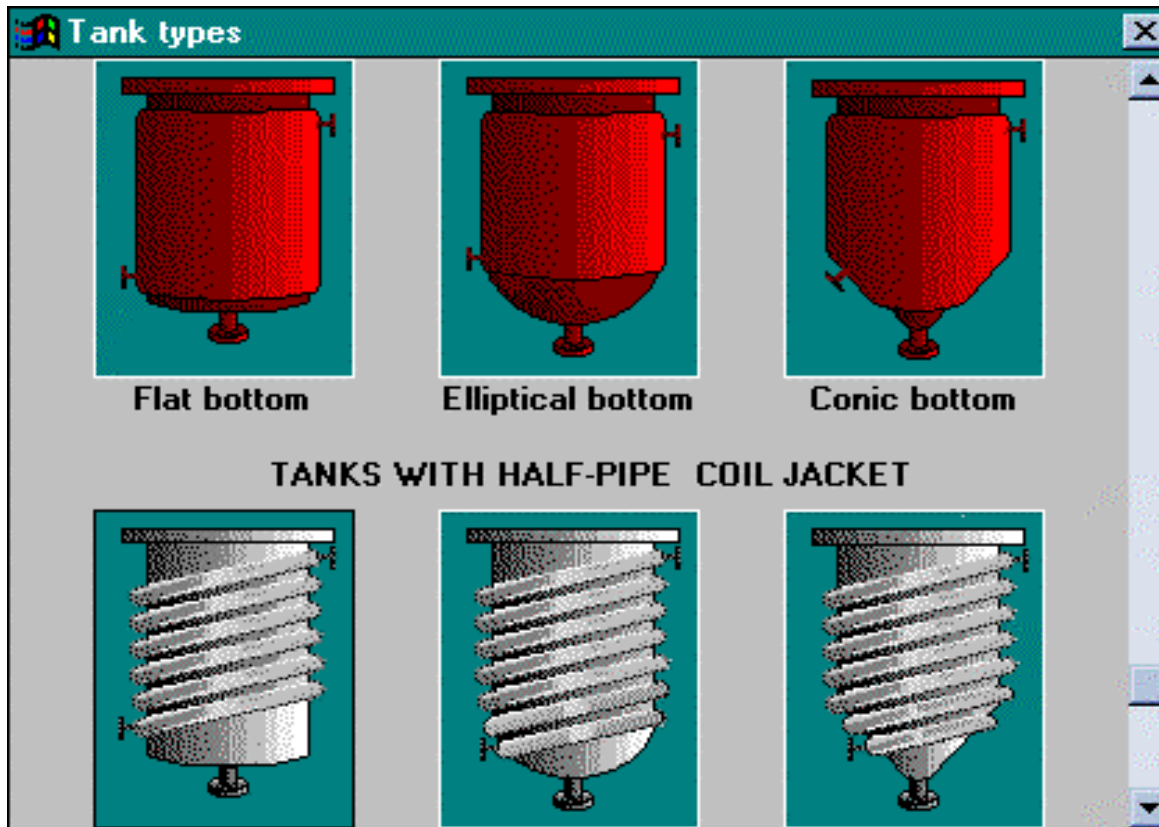
Liquid-gas mixing (gas dispersion)

Heat Transfer

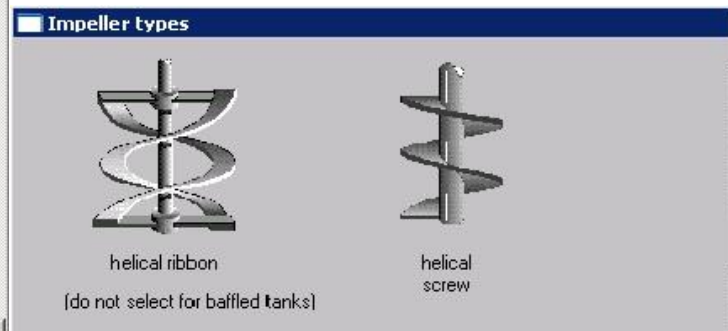
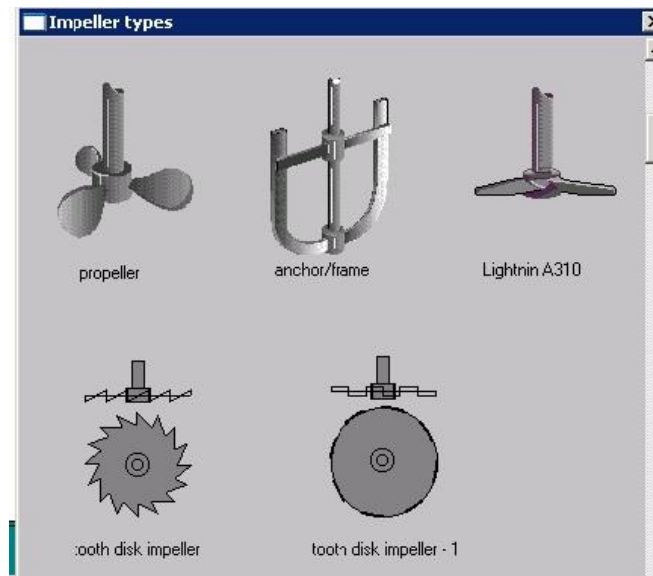
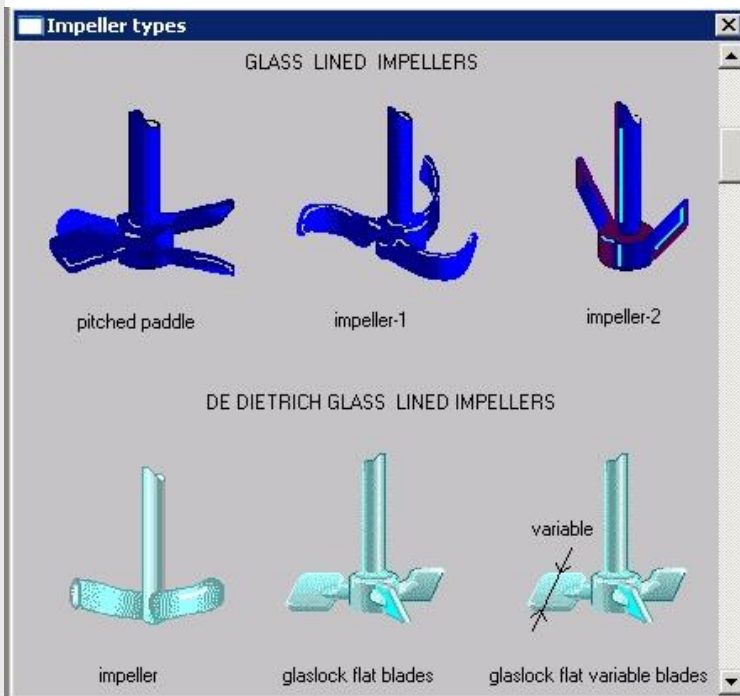
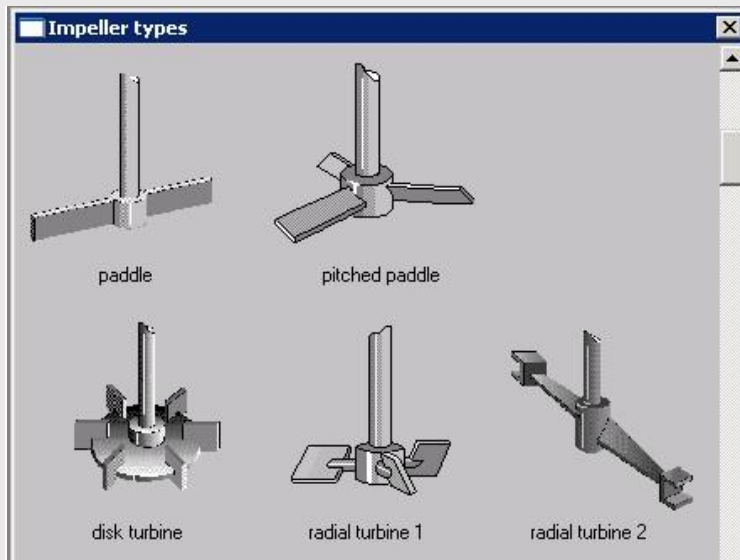
Mass Transfer in Liquid-solid systems

Mechanical Calculation of Shaft

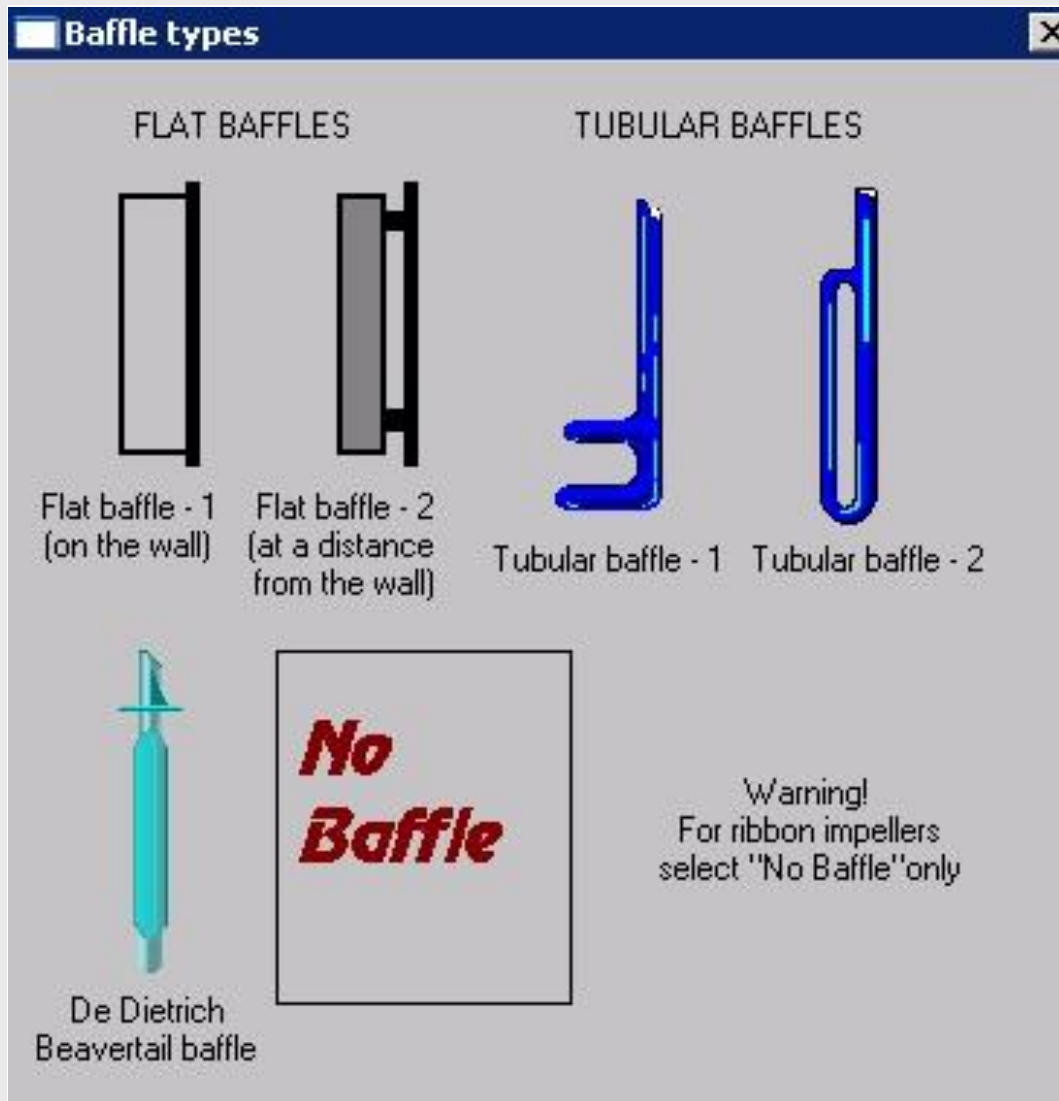
VISI MIX VESSELS/JACKETS



VISI MIX IMPELLERS



VISI MIX BAFFLES



- **Broad Range of Stirred Tank Mixing Problems**
- **Wide Variety of Impellers, Vessels and Baffles**
- **Scale/size**
 - **Lab, pilot, plant scale**
- **Hydrodynamic regimes**
 - **VisiMix Turbulent for flow Reynolds Number >1500**
 - **VisiMix Laminar for flow Reynolds Number < 1500**

ACCESSIBILITY OF

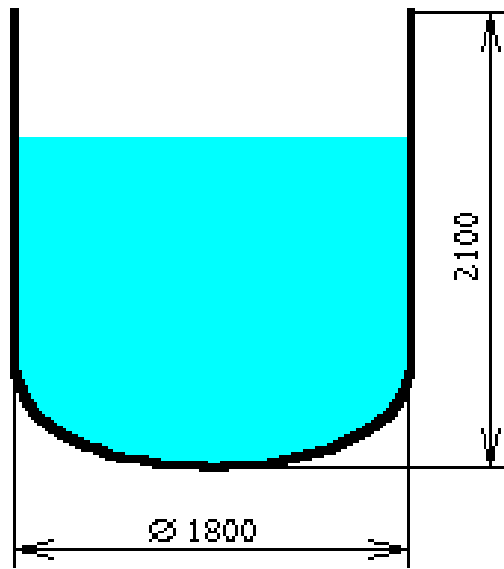


ACCESSIBILITY

E:\PROGRA~1\VISIMIX\VISIMIX3\DEM2.VSM

TANK WITH ELLIPTICAL BOTTOM

Inside diameter	<input type="text" value="1800"/>	<input type="text" value="mm"/> m ft mm micron in
Total tank height	<input type="text" value="2100"/>	<input type="text" value="l"/> mm in
Total volume	<input type="text" value="4962"/>	<input type="text" value="l"/>
Level of media	<input type="text" value="1525"/>	<input type="text" value="mm"/>
Volume of media	<input type="text" value="3499"/>	<input type="text" value="l"/>



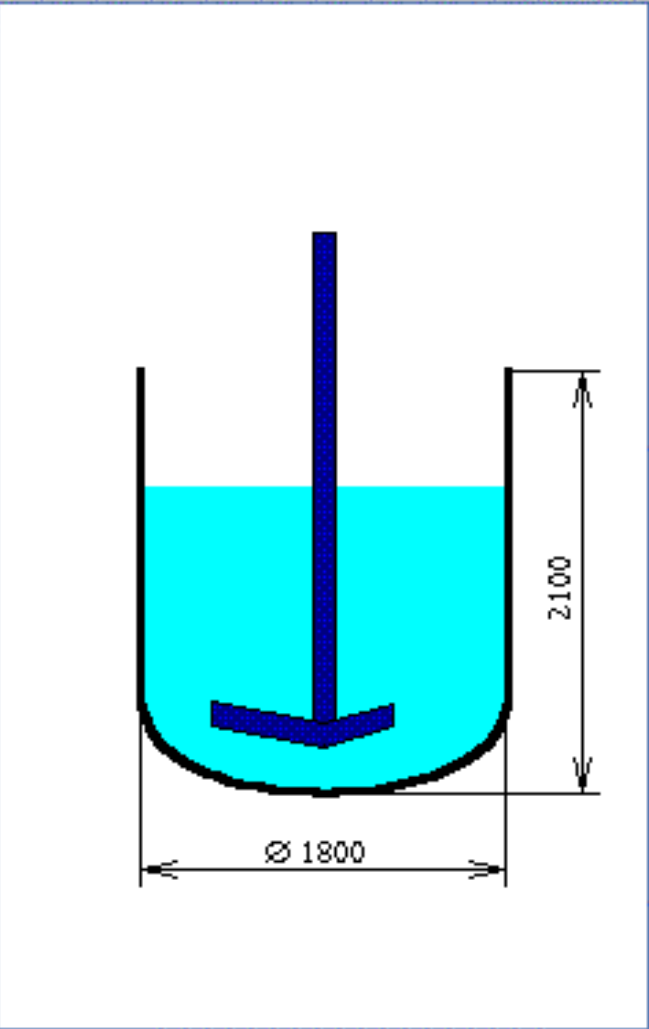
OK Cancel Choose new tank Print Help

ACCESSIBILITY

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PFAUDLER-2

Tip diameter	<input type="text" value="1100"/>	<input type="text" value="mm"/>
Number of blades	<input type="text" value="3"/>	
Width of blade	<input type="text" value="110"/>	<input type="text" value="mm"/>
Dist. from bottom	<input type="text" value="275"/>	<input type="text" value="mm"/>
Number of revolutions	<input type="text" value="100"/>	<input type="text" value="Rpm"/>
Power of drive	<input type="text" value="1500"/>	<input type="text" value="W"/>



OK Cancel Choose new agitator Print Help

ACCESSIBILITY

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FLAT BAFFLE-2

Number	<input type="text" value="4"/>
Width	<input type="text" value="152.4"/> <input type="text" value="mm"/>
Length	<input type="text" value="1981"/> <input type="text" value="mm"/>
Dist. from bottom	<input type="text" value="508"/> <input type="text" value="mm"/>
Dist. from wall	<input type="text" value="25.4"/> <input type="text" value="mm"/>
Angle to radius	<input type="text" value="0"/> <input type="text" value="deg"/>

OK Cancel Choose new baffle Print Help

ACCESSIBILITY

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AVERAGE PROPERTIES OF MEDIA

Type of media

 Newtonian Non-Newtonian

 Average density kg/cub.m

 Dynamic viscosity Pa*s

 Kinematic viscosity sq.m/s

 Constant K Pa*(sec)^{1-m}

 Exponent m

Behavior of Non-Newtonian media is approximated with the functions:

$$\tau = K * \gamma^{1-m}$$

$$\mu = K * \gamma^{-m}$$

 where μ - dynamic viscosity, Pa*sec;
 γ - shear rate, 1/sec;
 τ - shear stress, Pa.

OK

Cancel

Print

Help

ACCESSIBILITY

E:\PROGRAMS\VISIMIX\VISIMIX3\DEM2.VSM

PROPERTIES OF SOLID AND LIQUID PHASES.

Density of liquid phase	<input type="text" value="1000"/>	kg/cub.m
Dyn. viscosity of cont. phase	<input type="text" value="0.001"/>	Pa*s
Concentration of solid phase	<input type="text" value="150"/>	kg/cub.m
Density of solid phase	<input type="text" value="2500"/>	kg/cub.m
Average particle size	<input type="text" value="80"/>	micron
Size of largest particles *	<input type="text" value="300"/>	micron
Position of outlet-height	<input type="text" value="0"/>	mm

* significant fraction - 5% of solid phase

ACCESSIBILITY

E:\PROGRA~1\VISIMIX\VISIMIX3\DEM2.VSM

PROPERTIES OF CONTINUOUS AND DISPERSE LIQUID PHASES.

Continuous phase

Density kg/cub.m

Dynamic viscosity Pa*s

Disperse phase

Volume fraction

Density kg/cub.m

Dynamic viscosity Pa*s

Interfacial surface tension N/m

Index of admixtures

-1 - -0.5 - coagulants (de-emulsifiers)
 -0.5 - -0.1 - 2- and 3-valent ions of electrolytes
 -0.1 - 0.1 - no significant admixtures (pure oil - water)
 0.1 - 0.25 - electrolytes
 0.25 - 0.5 - small quantities of detergents
 0.5 - 1 - detergents, emulsifiers

OK Cancel Print Help

ACCESSIBILITY

E:\PROGRA~1\VISIMIX\VISIMIX3\DEM2.VSM

**SINGLE PHASE BLENDING AND REACTORS.
HOMOGENEOUS CHEMICAL REACTION**

MAIN REACTION A + B = C Reactant A charged initially to the tank	SIDE REACTION Side reaction is assumed to be slow compared to the main reaction
Specific reaction rate for BLENDING - enter 0 (zero) for FAST reaction - enter F	Reaction type
<input type="text" value="F"/> l/(mol*sec)	<input type="text" value="B + C = D"/>
Init. concentration of reactant A	Specific reaction rate
<input type="text" value="0.8"/> mol/liter	<input type="text" value="0"/> l/(mol*sec)
Relation of loads - B[mol]/A[mol]	
<input type="text" value="1.03"/>	

OK Cancel Print Help

ACCESSIBILITY OF



INTERFACE: Simple, Intuitive, Context-Relevant Interface

- **Input data: equipment dimensions, fluid properties, process or operational parameters**
- **SI or US Customary Units**
- **Fast Solver**
- **Values of Relevant Hydrodynamic, Turbulent and other Mixing parameters returned**
- **Desired process result IS NOT an Input**

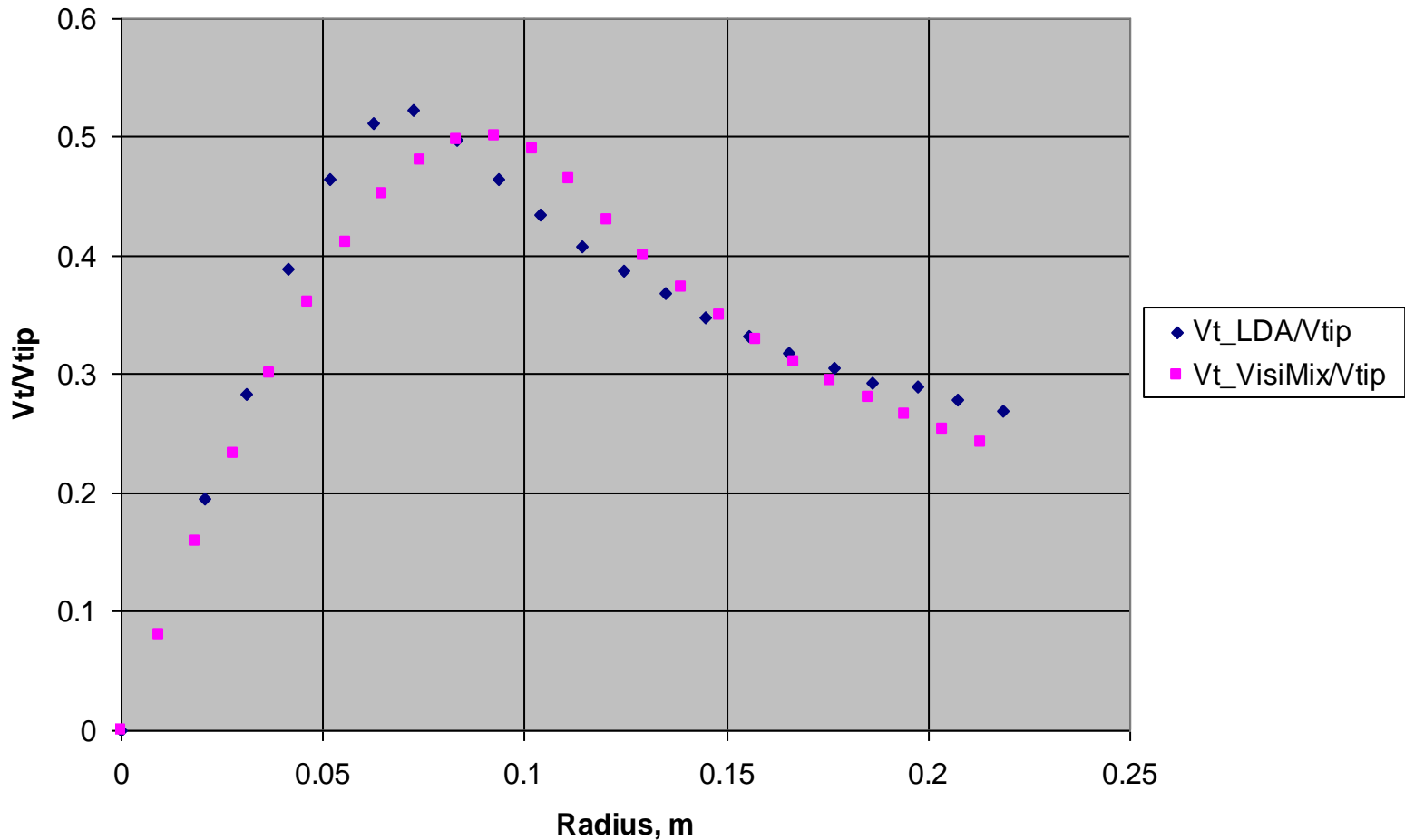
RELIABILITY OF



- **Comparison with**
 - **data**
 - **established correlations**
- **Magnitude as well as functional dependence on key properties and parameters**

RELIABILITY

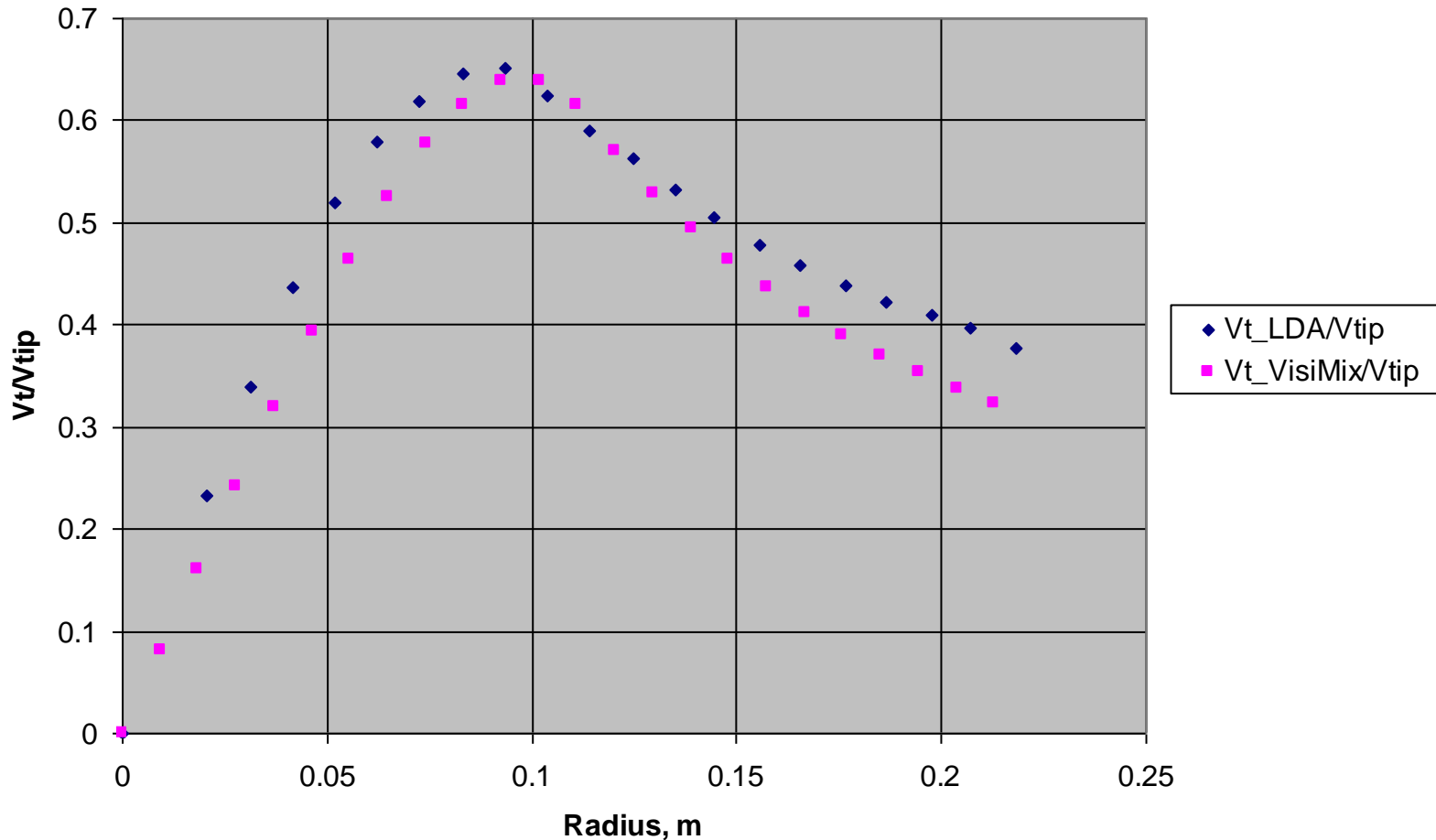
Radial Distribution of mean tangential velocity
PBT4-9" @ 150 rpm in unbaffled vessel
 LDA Data by S.P. Wood & K. Barton, 1993



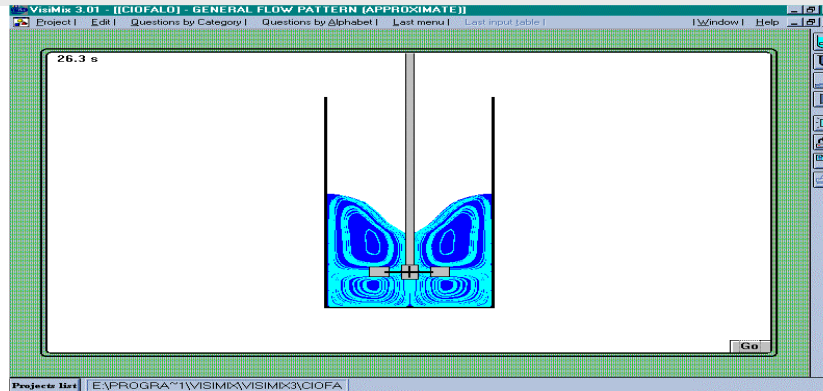
RELIABILITY

**Radial Distribution of mean tangential velocity
DT6-9" @ 150 rpm in unbaffled vessel**

LDA Data by S.P. Wood & K. Barton, 1993



RELIABILITY



Ref.: Ciofalo, M. et al (1996) “Turbulent flow in Closed and Free-surface Unbaffled Tanks Stirred by Radial Impellers”, Chem. Eng. Sci. 51 (14), pp 3557-3573.

	Measured data	VisiMix Results
Vortex Depth @ 139 rpm, m	0.026	0.024
Vortex Depth @ 194 rpm, m	0.047	0.047
Vortex Depth @ 240 rpm, m	0.073	0.073

RELIABILITY

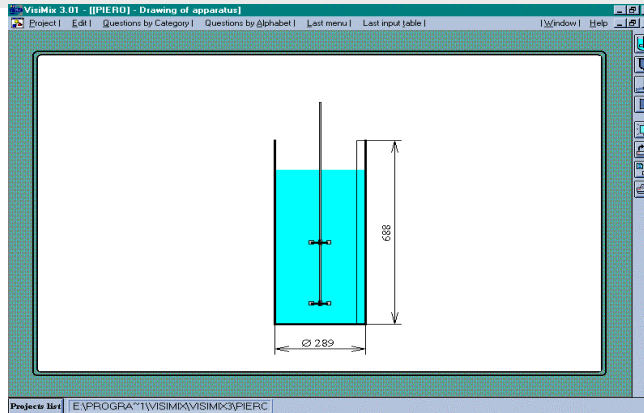
System: Water

T=78 in, H=T, D=T/3, C=T/3, 4 Std. Baffles, N=125

	<u>RDT</u>	<u>PBT</u>	<u>A310</u>
Power Number, P_o	4.71 5.2	1.67 1.31	0.29 0.3
Ave. Specific Power, W/kg	0.78 1.0	0.28 0.26	0.06 0.06
Mixing time 99%, s	15 23	16 36	31 -

Note: Results calculated with correlations from BHRG-FMP in shaded bold italics

RELIABILITY



Ref.: Armenante, P. M. And Chang, G. (1998) “Power Consumption in Agitated Vessels Provided with Multiple Disk Turbines”, Ind. Eng. Chem. Res. 37, pp.284-291.

Two Rushton turbines	Measured data	VisiMix Results
Power Number @ $S=D$	7.5	9.9
Power Number @ $S=3D$	9.6	10.8

RELIABILITY

Ref. Harrop et al (1997) "Impact of suspended solids on the homogenisation of the liquid phase under turbulent conditions in a stirred vessel", Proceedings of Mixing IX,

Paris: Recent Adv. in Mixing 11 (52), pp41-48

System: Water, T=720 mm, H=T, 4 Std. Baffles

A315, D/T=0.42, C=T/4

N, rpm	W/kg Expt.	W/kg VisiMix	Mixing time, s Conducti- vity	Mixing time, s Decolori- zation	Mixing time, s BHRG- FMP	Mixing time, s VisiMix
100	0.038	0.035	19.3	26.6	19.0	24.8
150	0.128	0.117	12.3	16.7	12.7	16.6
200	0.293	0.278	9.3	11.5	9.6	12.4
250	0.544	0.542	7.3	10.0	7.8	9.92
300	0.921	0.937	7.3	8.0	6.5	8.27
350	1.421	1.490	6.7	7.5	5.7	7.09
400	2.123	2.223	5.3	5.8	5.0	6.2

Note: VisiMix Results courtesy of Dr. Braginsky

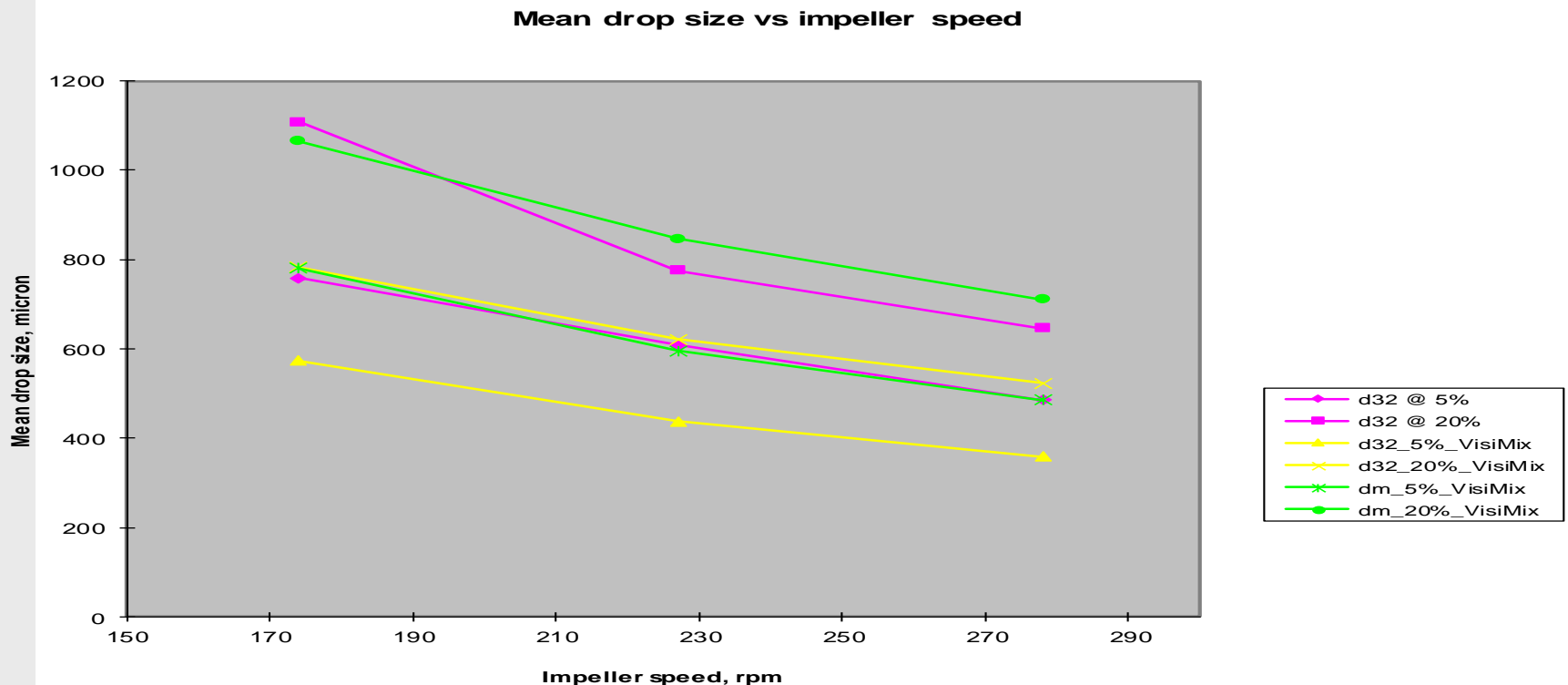
RELIABILITY

Ref.: Ross, et al. (1978) "Droplet Breakage and Coalescence Processes in an Agitated Dispersion. 2. Measurement and Interpretation of Mixing Experiments", Ind. Eng. Chem. Fundam., 17 (2) pp 101-108

Liquid/Liquid: 39.1% v Dowtherm E, 61.9% v Shell No. 3747 Oil/Water Vessel: T=11.1 cm Impeller: RDT, D/T=0.46, C=T/3	Data	VisiMix Results	VisiMix Results
	d_{32} μm	d_{32} μm	d_{mean} μm
@ 5.0 % (v) dispersed phase, N=174	758	781	574
@ 5.0 % (v) dispersed phase, N=227	608	596	438
@ 5.0 % (v) dispersed phase, N=278	486	486	358
@ 20.0 % (v) dispersed phase, N=174	1108	1065	783
@ 20.0 % (v) dispersed phase, N=227	775	847	622
@ 20.0 % (v) dispersed phase, N=278	646	711	523

RELIABILITY

Ref.: Ross, et al. (1978) "Droplet Breakage and Coalescence Processes in an Agitated Dispersion. 2. Measurement and Interpretation of Mixing Experiments", Ind. Eng. Chem. Fundam., 17 (2) pp 101-108



RELIABILITY

- **Reasonable match with data or results from established correlations in several selected cases**
- **Acceptable trends in calculated values**
- **Some results deviate significantly from data and results from established correlations**

VisiMix as an Engineering Productivity Tool

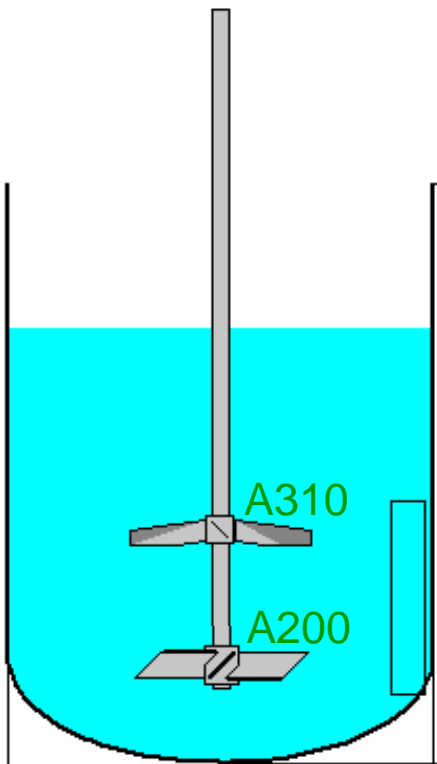
- + Simple, Intuitive, Context-Relevant
- + Useful for characterizing and comparing well defined mixing systems
- + No other tool with similar coverage!
- Rating tool NOT design tool



VISI MIX APPLICATION CASE # 1

Troubleshooting

Modified agitation setup to improve powder drawdown



Process Loads: 5200

gal liquid

7400 lbs powder

The problem:

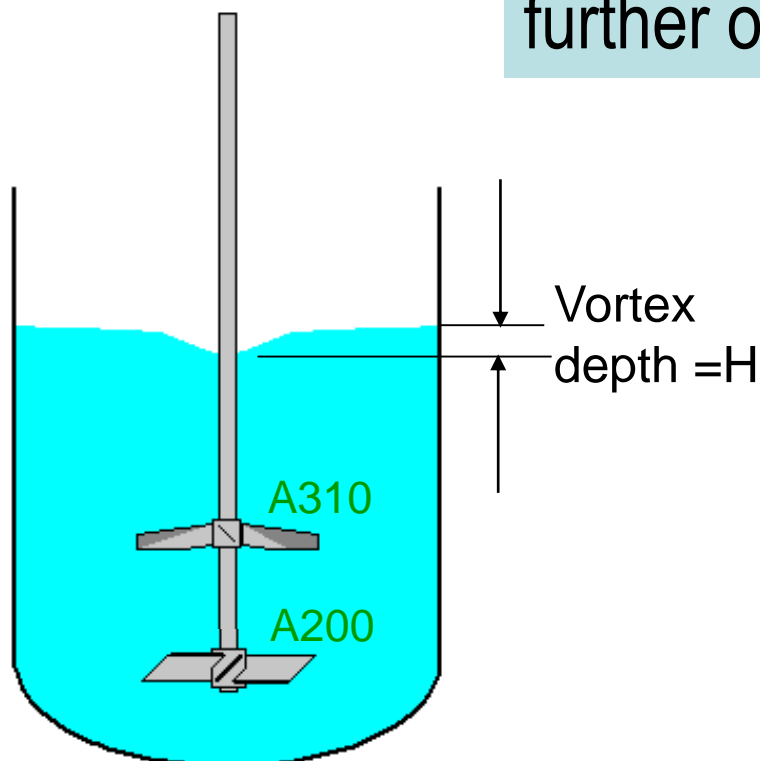
- Poor mixing due to problem with powder drawdown

Constraints:

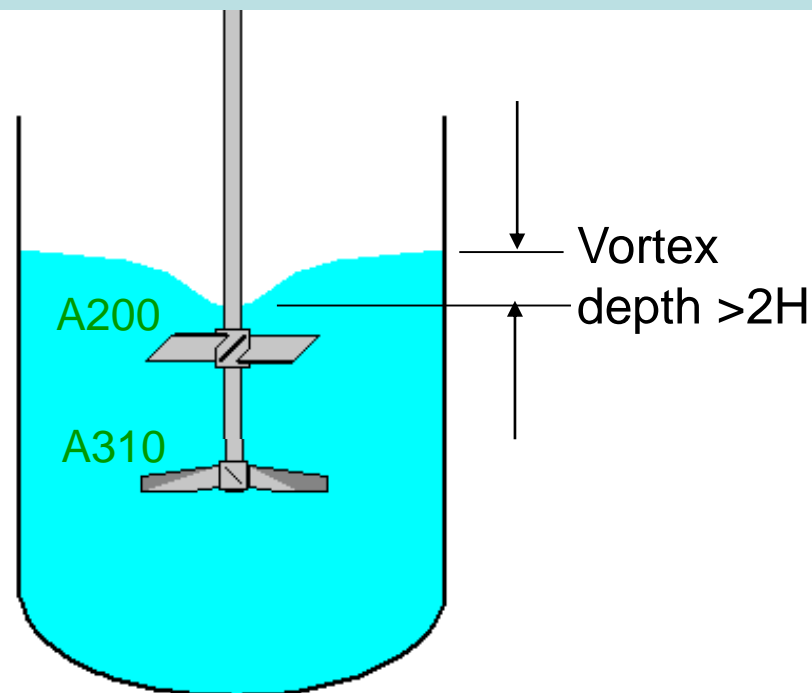
- Impeller already operated at maximum rotation speed (RPM)
- Solution required to avoid risks of powder attrition
- Air entrainment is undesired for process

VISIMIX APPLICATION CASE # 1

Modification ideas tested / evaluated and further optimized in VISIMIX



Previous setup



Modified setup

- Switch upper/lower impeller to let A200 (with much higher flow # than A310) at the top
- New positions of both impellers **optimized by VISIMIX** for maximum powder drawdown but without causing gas entrainment
- Maintain same shaft RPM to avoid risk of powder attrition
- **Implementation:** successful modification with almost zero capital

VISI MIX APPLICATION CASE #2

Scale-up from lab to commercial production



Liquid volume: 700 cc
Liquid weight: 0.6 kg

Problem definition:

Scale up to the commercial production of 6000 kg per batch (10,000 times!!)

-- What reactor to choose?

choose from a few available/idle vessels & agitation systems to reduce capital

-- How to scale up agitation?

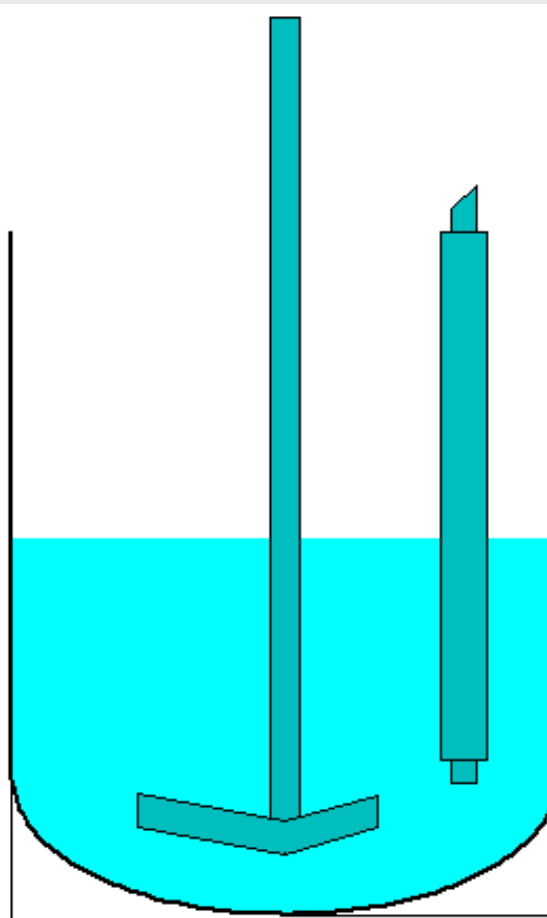
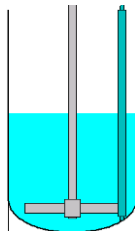
lab tests showed that the product quality was very sensitive to mixing or agitation. Too much or too little agitation would negatively affects product

-- What is the mixing time?

VISIMIX APPLICATION CASE #2

Scale up by 10,000 times
with VISIMIX

Lab Reactor:
Batch size: 700 cc
Batch weight: 0.6 kg

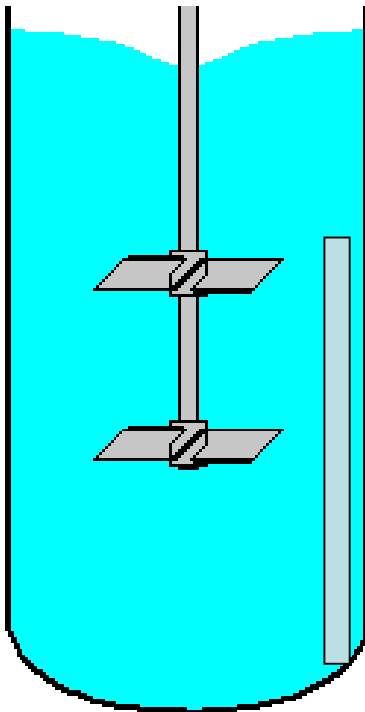


Commercial production
Reactor:
Batch size: 7 m³
Batch weight: 6000 kg

Scale-up by mixing power per unit mass:

- Simulate the lab setup to obtain “mixing power per unit mass”
- Simulate the commercial production with available vessels and agitation systems, adjust the impeller speed to match the “mixing power per unit mass”
- Verify mixing time
- Successful scale-up implementation

VISIMIX predicts surface vortex and exports to CFD



Liquid volume 18 m³
Liquid level above baffles

Most CFD simulations of stirred tank ignore surface vortex

- flat surface assumed, usually OK for fully baffled tank

Surface vortex effect needs to be included in CFD *if*

- near-surface hydrodynamics is critical (e.g., powder drawdown)
- the tank is not fully baffled

Directly modeling the free surface in CFD significantly increases the complicity and cost of CFD simulations

- turn single-phase flow into 2-phase flow, or
- turn 2-phase flow into 3-phase flow,
- turn steady-state flow into transient flow simulation (sliding mesh)

Use VISIMIX to predict the free surface (surface vortex)

Export the free surface geometry into CFD which is used as the domain top boundary specified with “slippery-wall” condition

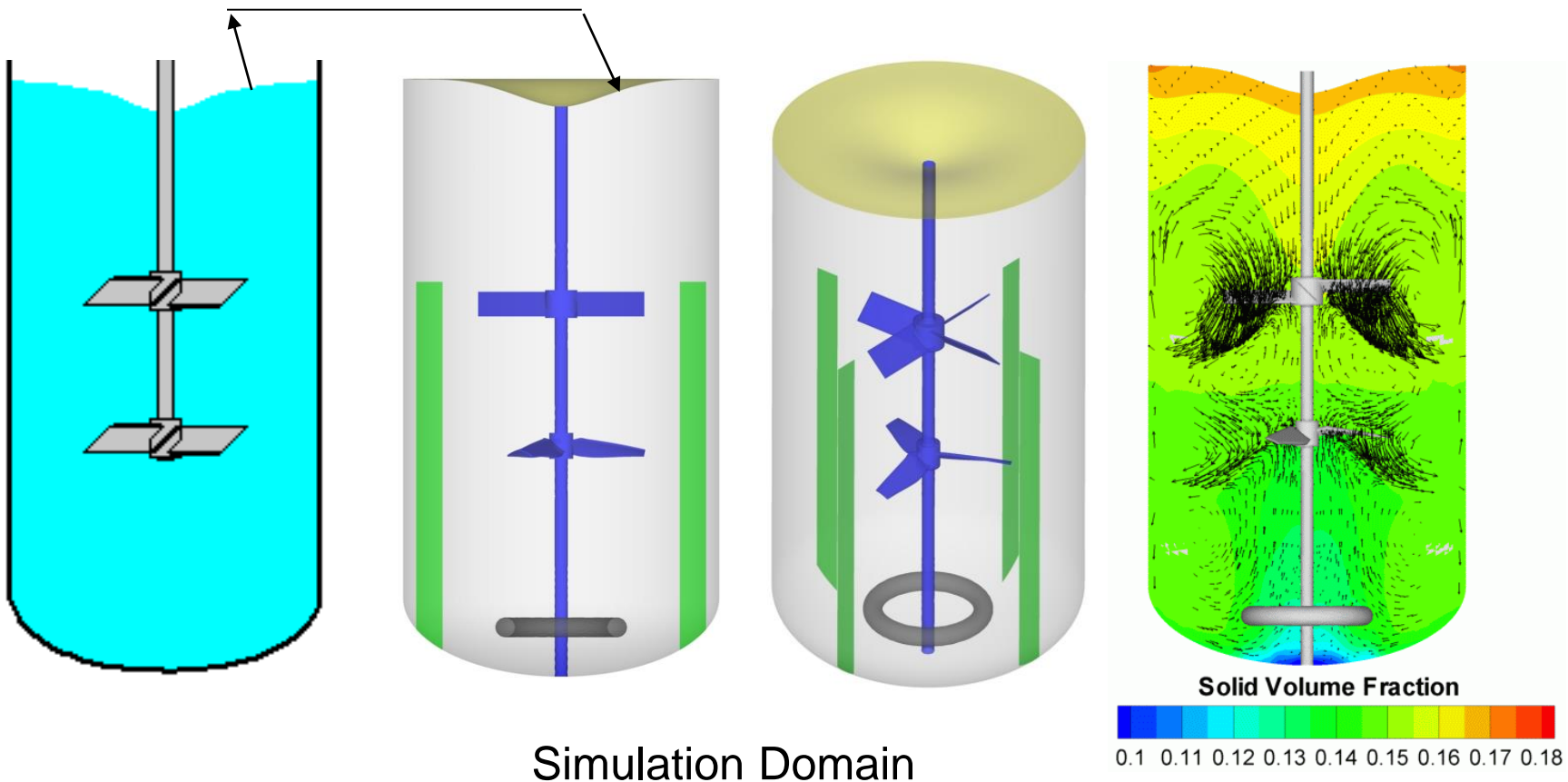
This approach significantly improves efficiency of CFD simulations with reasonable approximation of the surface vortex

VISIMIX APPLICATION CASE #3

VISIMIX

CFD

CFD domain top boundary based on VISIMIX prediction



VISIMIX APPLICATION CASE #4

comparing VISIMIX and lab experiments

Laboratory system to measure axial distribution of heavy solids

chemical system

40 wt% solids in NaCl

60 wt% salt tap water

2 g NaCl / kg tap water

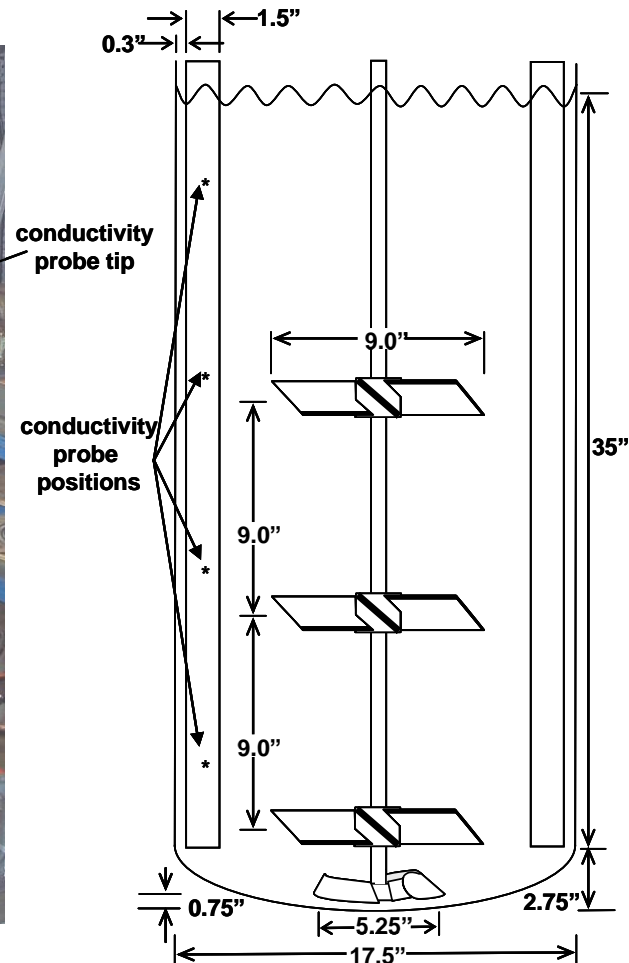
Property of solid spheres

$$\rho_{app} = 1.7 \text{ g/cc}$$

$d_p = 285 \text{ } \mu\text{m}$ vol. med.

(<1 wt% 15-100 μm)

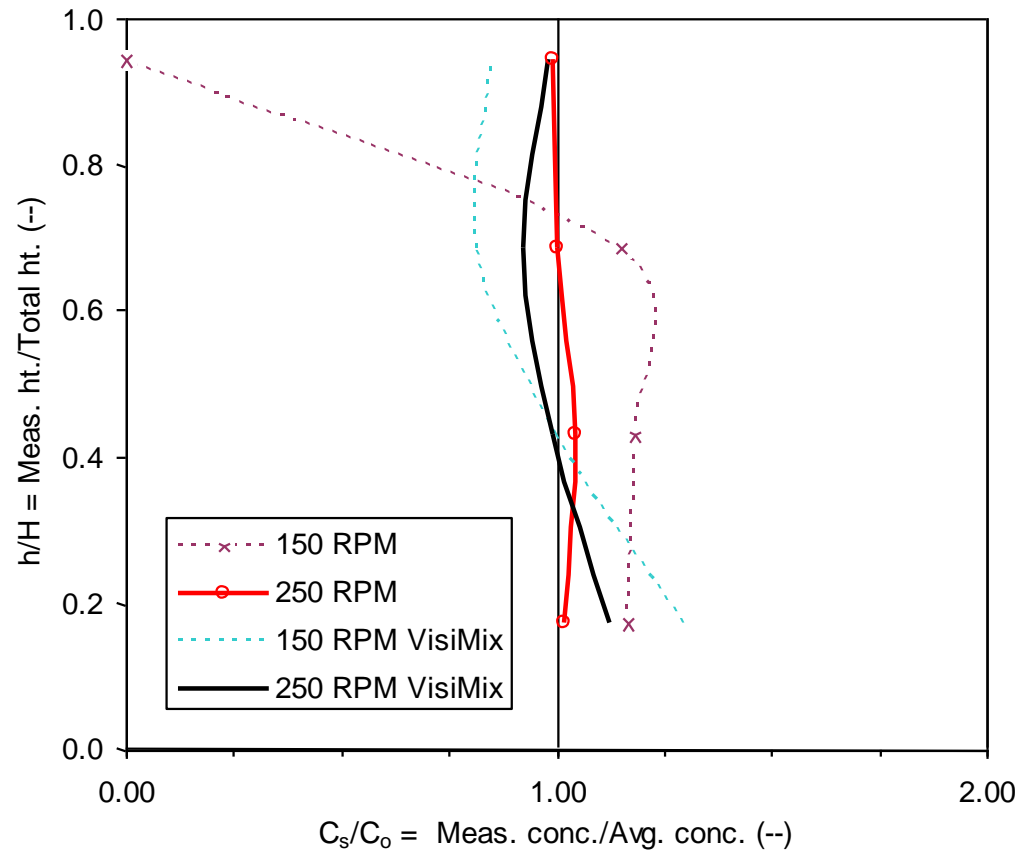
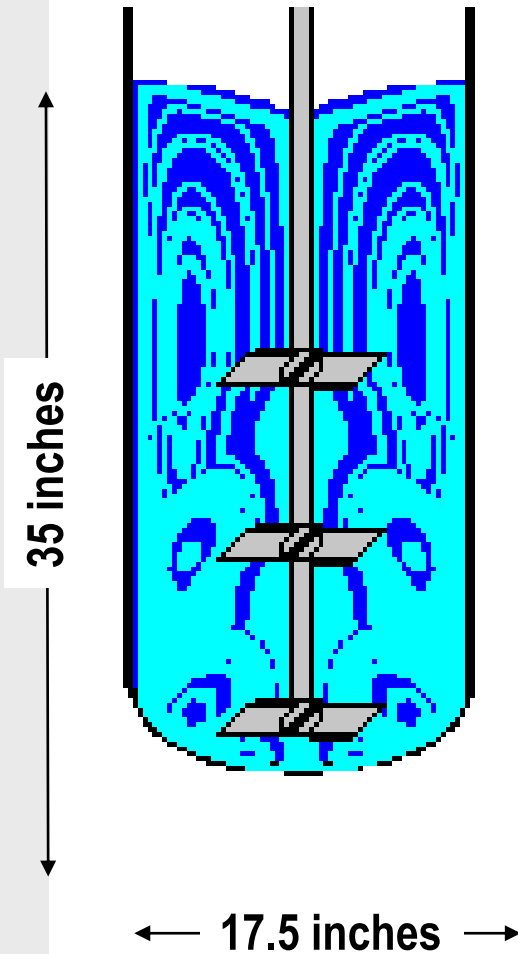
(<1.5 wt% 425-600 μm).



VISI MIX APPLICATION CASE #4

Normalized, axial solids distribution VisiMix vs. measured

Simulation: three standard PBTs



Mixing Problem Solving

Key questions for process development

- What is success for the desired process?
- How does mixing affect the desired process?
- What kind of mixing will achieve success for process?
- What kind of mixing will hurt the process?
- When and why is it important?
- What measures characterize the effects?
- How important are the effects on the process?
- What equipment design and/or operations will produce the desired process result?



Summary

Focus on achieving desired process result

- *Link “effective mixing” to achieving desired process result*

Describe effective mixing in terms of

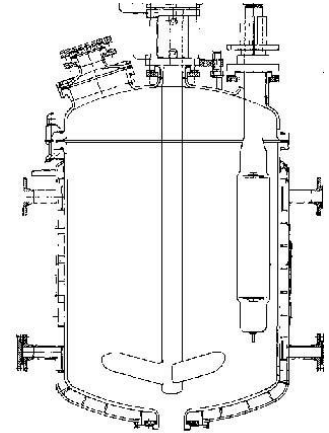
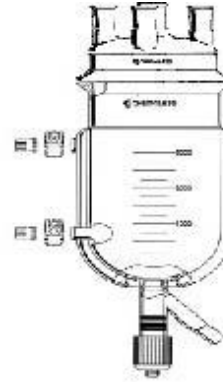
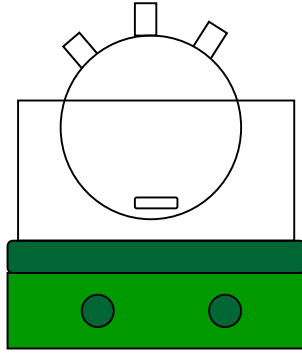
- *required hydrodynamics and relevant physicochemical phenomena necessary for process success*
- *confirm with basic calculations, experiments and/or modeling*

Recommend/select equipment and/or operating conditions to achieve desired process result

Ascertain reliability of mechanical design



Process R&D and Scale-up Factors



Physical properties

- Phases
- Density
- Viscosity & rheology

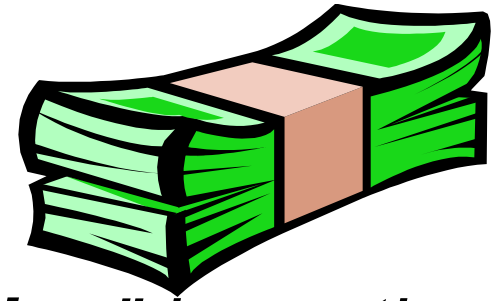
Chemistry

- Chemical equilibria
- Chemical kinetics

Transport phenomena

- *Hydrodynamics/Mixing*
- Mass transfer
- Heat transfer

IMPORTANT LESSONS



Process failure from “inadequate mixing” is costly

- lower reaction yields, more by-product formation
- longer reaction/process times
- unacceptable product properties
- higher costs for purifications, waste handling, etc.
- higher production costs for product rework, etc.
- less safe operations

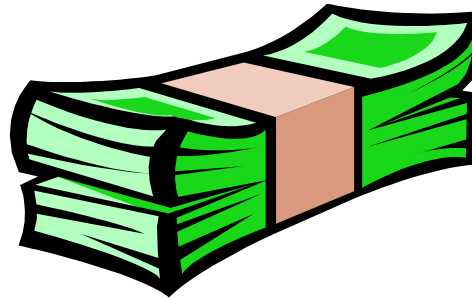
Early and careful assessment of effect of mixing on process is imperative!



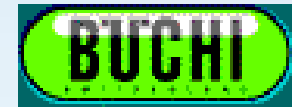
Key Message

Early assessment of effect of mixing on process is essential!

- **Cost to make changes is lower**
- **Opportunity is higher to**
 - **influence process decisions**
 - **avoid /prevent process scale-up problems !!**
 - **achieve process goals**
 - **make money**



Customers and Markets



Customers and Markets

- 1.3M, USA
- 2.Afton, USA
- 3.Air Products, USA
- 4.Alkermes
- 5.AllessaChemie
- 6.ASEPCO
- 7.Ashland Hercules
- 8.BASF, USA
- 9.Belinka Belles
- 10.Celgene
- 11.Chemagis
- 12.DeDietrich
- 13.Dow Chemical Company
- 14.Eni - Milan
- 15.Evonik Degussa
- 16.GE Technologies
- 17.GE Healthcare
- 18.Global Tungsten & Powders
- 19.Honeywell-UOP
- 20.Ineos Styrenics
- 21.Lubrizol
- 22.Merck - Schering-Plough
- 23.Mitsubishi
- 24.NALAS-Jerry Salan
- 25.Nan Ya Plastic
- 26.Nippon
- 27.Novartis
- 28.NRDC, India
- 29.Ocean
- 30.Pfizer
- 31.Polimeri
- 32.Praxair
- 33.Ranbaxy
- 34.Samsung, Korea
- 35.Sunovion Sepracor
- 36.SES
- 37.Solvay
- 38.Tecnicas Reunidas
- 39.Tecnimont, Italy
- 40.Teva Global
- 41.US Navy, USA
- 42.Alcon, USA
- 43.Arizona Chemical
- 44.JM Huber
- 45.Jotun
- 46.Lek
- 47.Matrix\Mylan
- 48.MJN - Mead Johnson Nutrition
- 49.Ranbaxy
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- 55.Ash Stevens Inc.....

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Thank You!