VisiMix – Productivity Tool for the Analysis, Scale-up and Design of Mixing Processes in Stirred Tanks

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PROCESS DEVELOPMENT & SCALE-UP

PROCESS DEVELOPMENT & SCALE-UP

Engineer/ Chemist Interface Opportunities

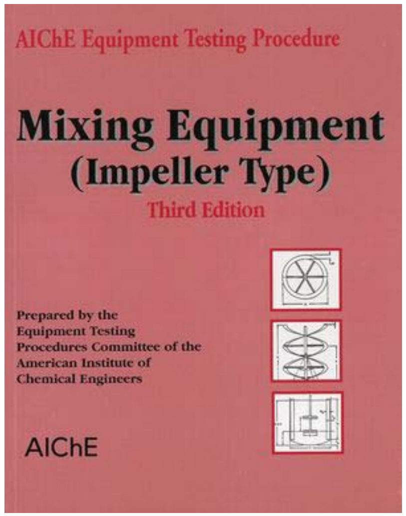
- Reaction Chemistry
- Technology Development
- Minimum Scale Up Issues
- Mixing Phenomena
- Heat Transfer/ Heat of Reaction
- Kinetic Modeling
- Particle Formation and Control
- Distillation/ Recycle/ Purification
- Liquid/ Liquid (Phase) Separation
- Solid/ Liquid Separation

Important lesson for Process Development

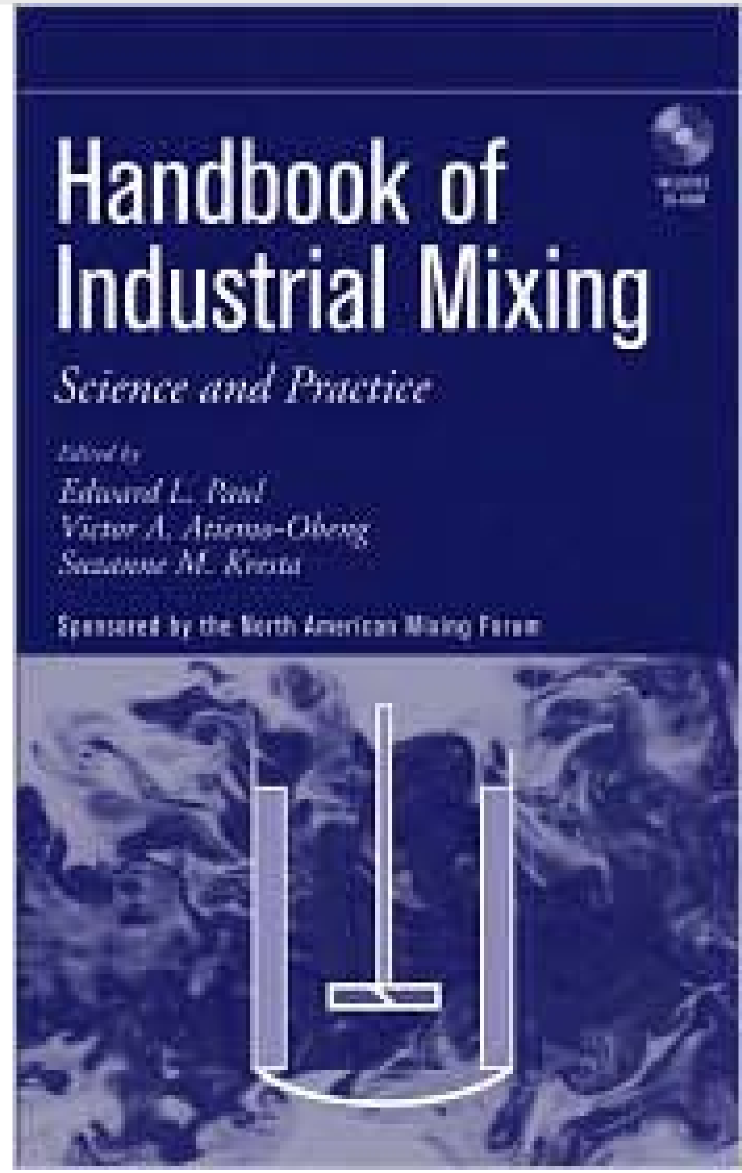
Early assessment of effect of mixing on process

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

RESOURCES



Dickey, D., et al (2001) **AIChE Equipment Testing Procedure - Mixing Equipment (Impeller Type), 3rd Edition**



Key Steps in Process / Mixing Consulting & Problem Solving

Define the correct problem to be solved

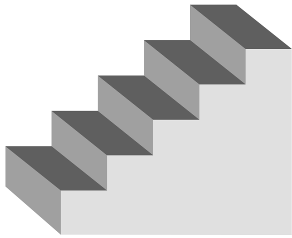
- Establish mixing objective/**desired process result**

Perform analysis

- **Determine required hydrodynamic environment and operating conditions, relevant physicochemical phenomena and controlling parameters necessary for process success**
- **Confirm with basic calculations, experiments and/or modeling**

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

Ascertain reliability of mechanical design



Mixing Processes:
Key Variables to explore

Effects of

- impeller geometry (type, size, etc.)
- impeller speed (rpm)
- feed location (sub-surface, near impeller)
- feed time in semi-batch
- feed concentration
- temperature
- fluid viscosity
- Etc.

Mixing Problem Solving

Process engineer asks-

- What kind of mixer?
- Which impeller type?
- How many impellers?
- What's impeller speed?
- What's motor horsepower?
- What's size of gear box?
- Etc.

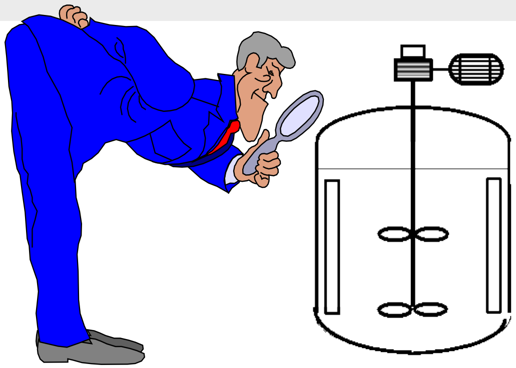
Good questions but ...

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?

Need for Mixing Productivity Tool



Effective capture and use knowledge of

- mixing phenomena
- fluid mechanics
- characteristics of mixing equipment, etc.

at different levels of sophistication

to quickly analyze, scale-up, design, troubleshoot mixing processes in stirred tanks.

Relevance of

VisiMix

Relevance of VisiMix

MIXING ASPECTS COVERED:

Hydrodynamics

Turbulence

Single phase Mixing (Blending & Reaction)

Batch, Semi-Batch, Continuous

Liquid-Solid mixing

Liquid-liquid mixing (liquid dispersion)

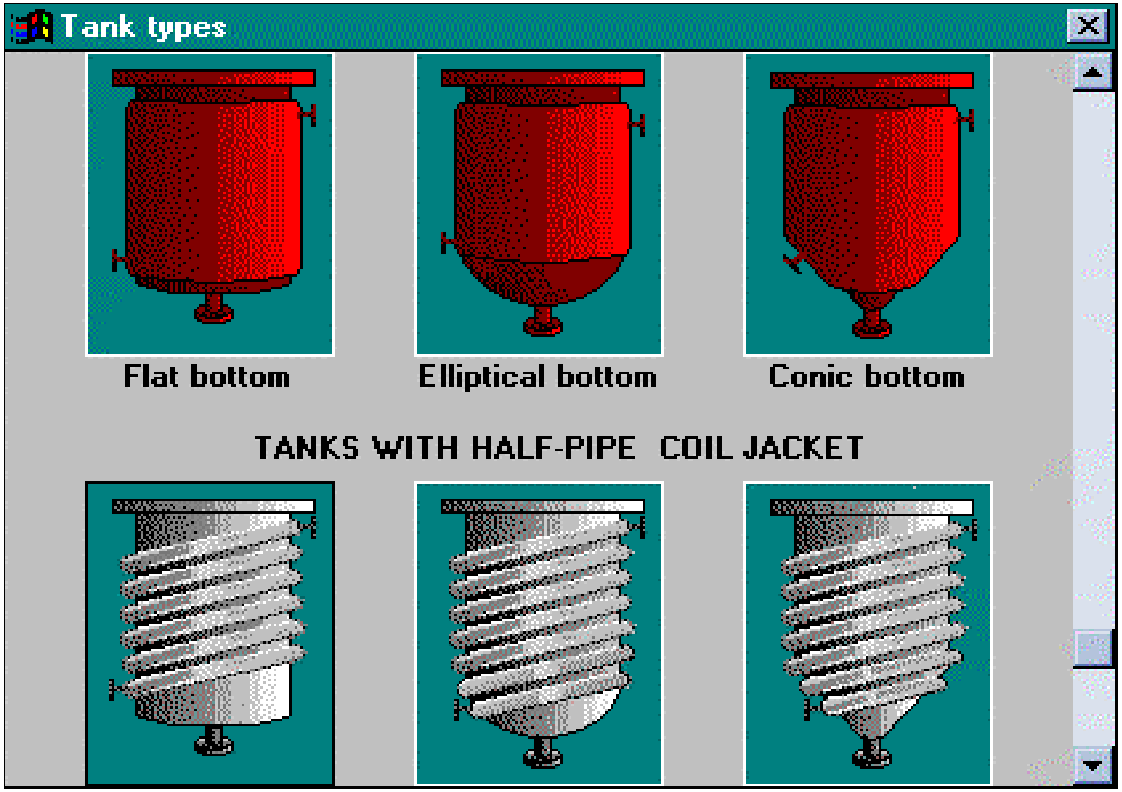
Liquid-gas mixing (gas dispersion)

Heat Transfer

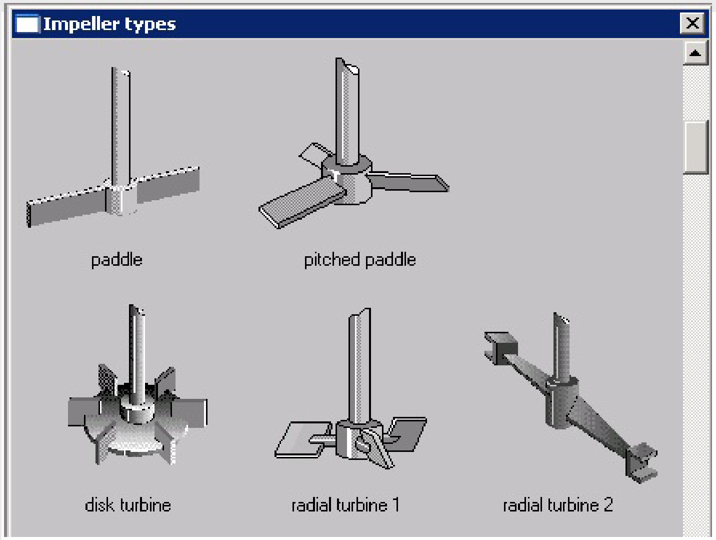
Mass Transfer in Liquid-solid systems

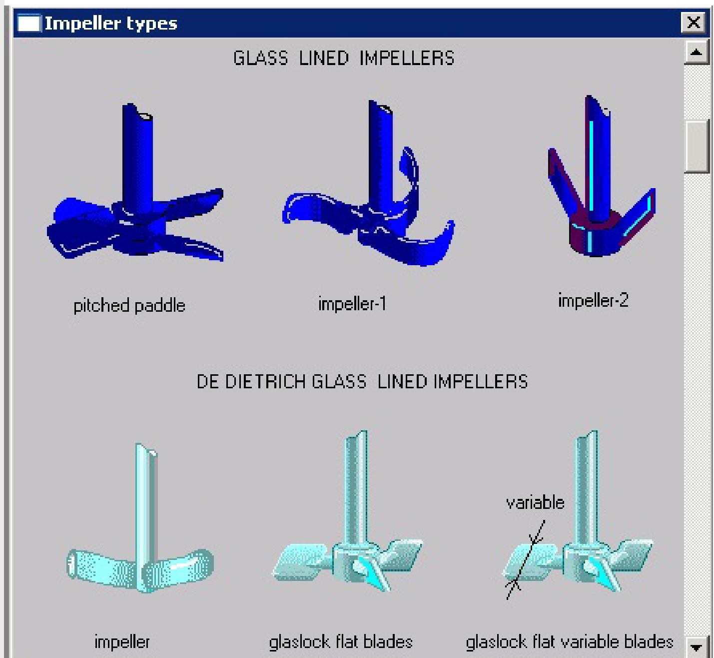
Mechanical Calculation of Shaft

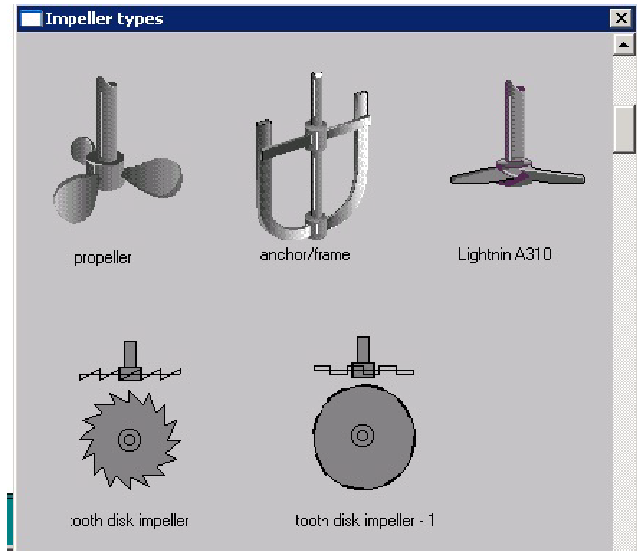
VisiMix Vessels/Jackets

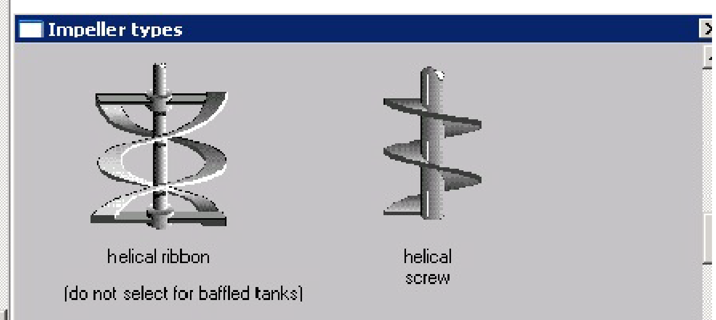


VisiMix Impellers

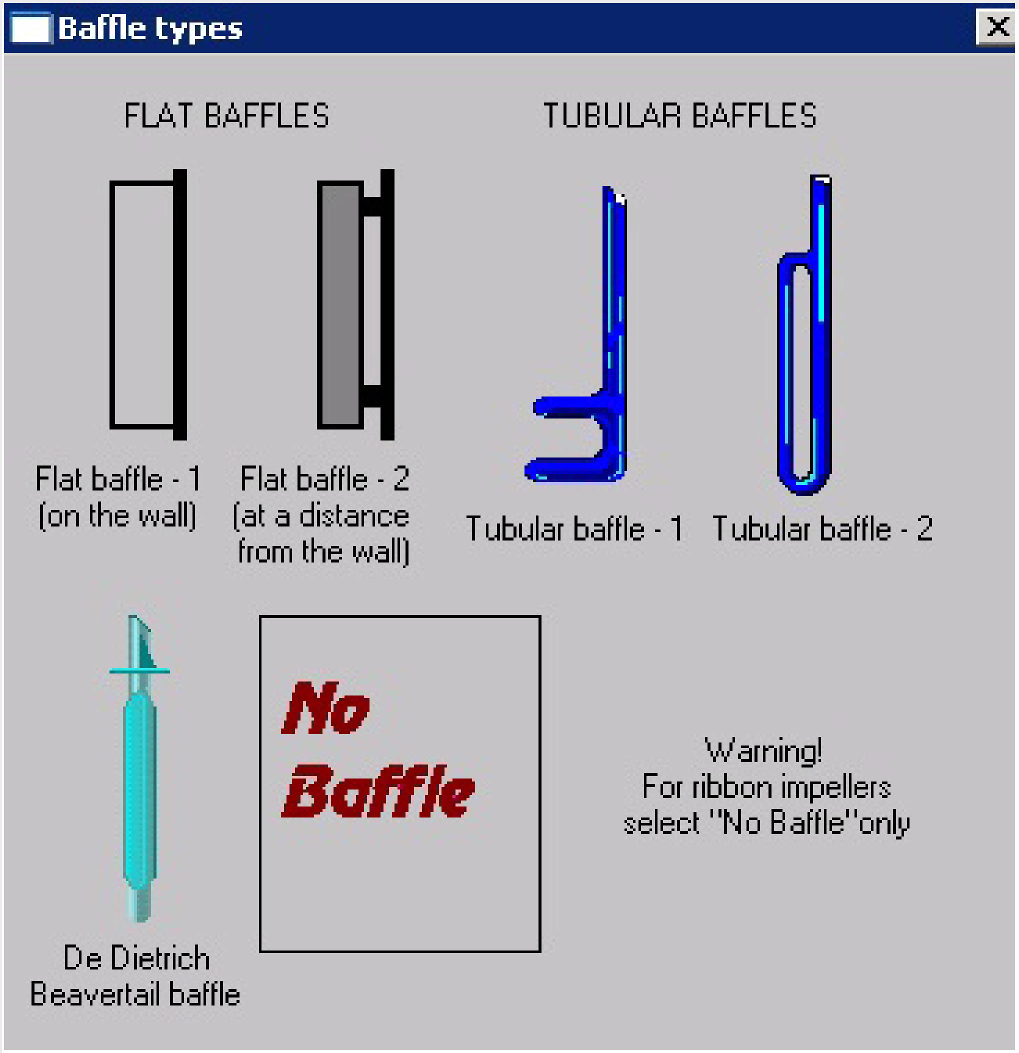








VisiMix Baffles



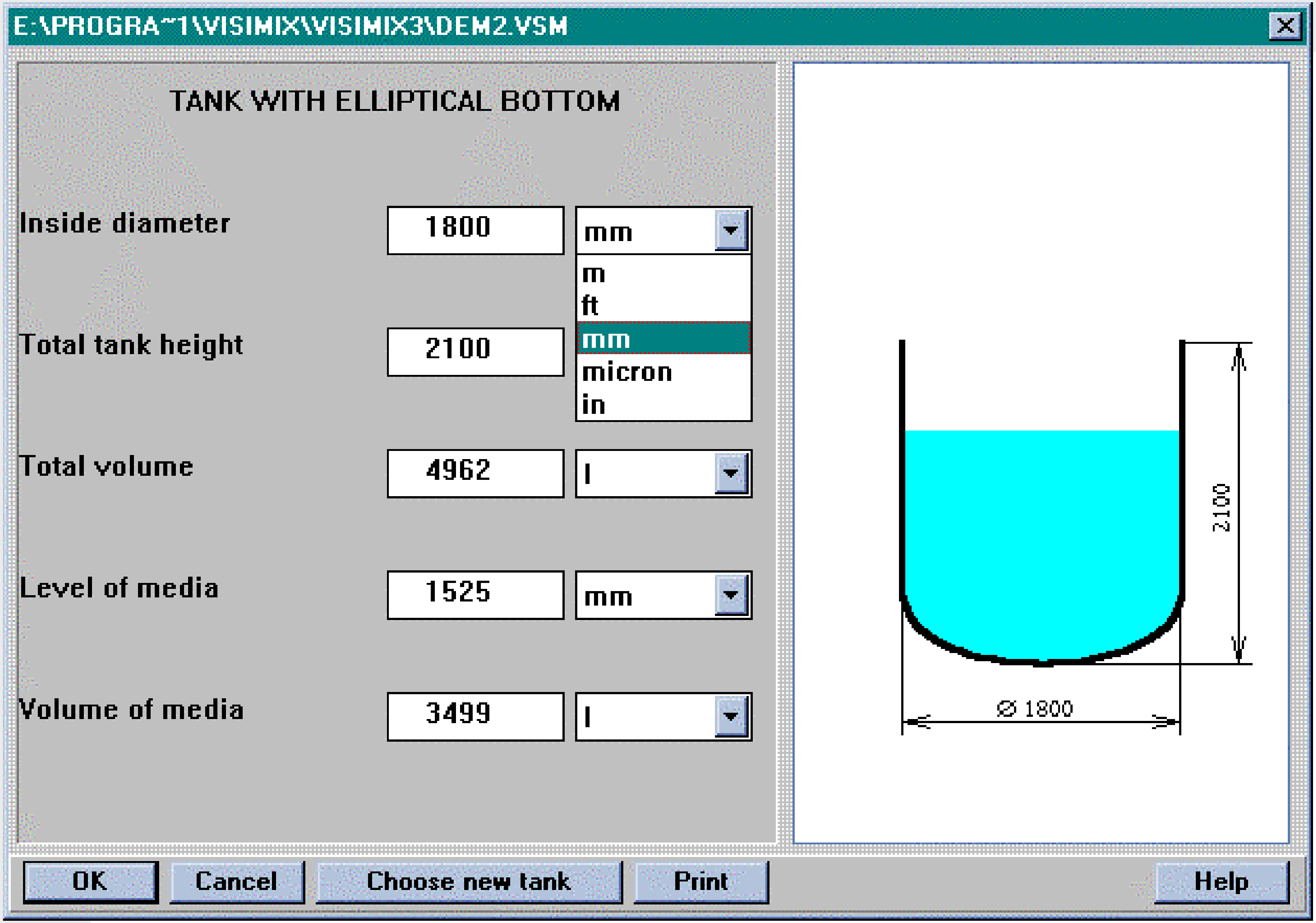
RELEVANCE OF VisiMix

- 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

VisiMix

ACCESSIBILITY



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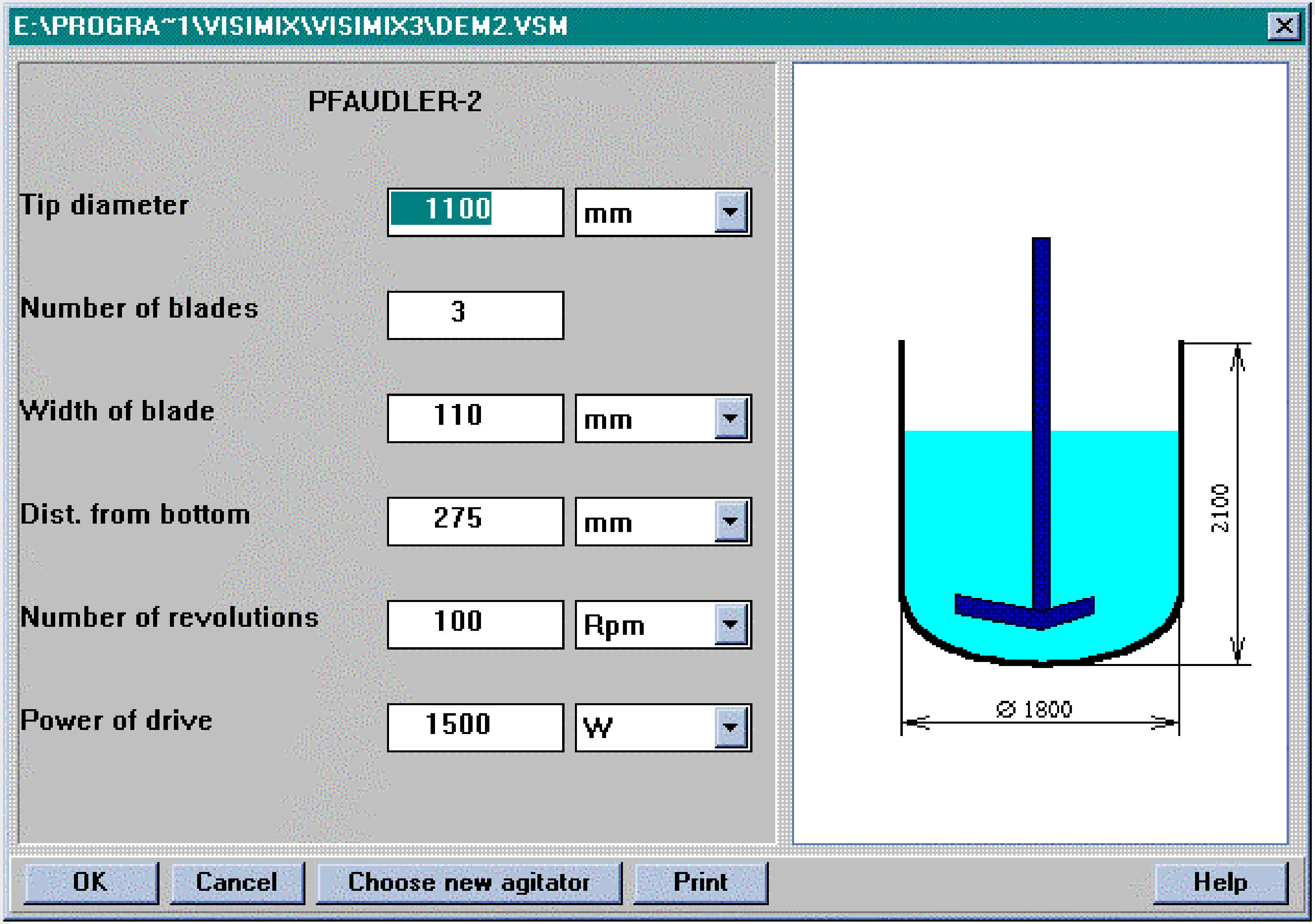

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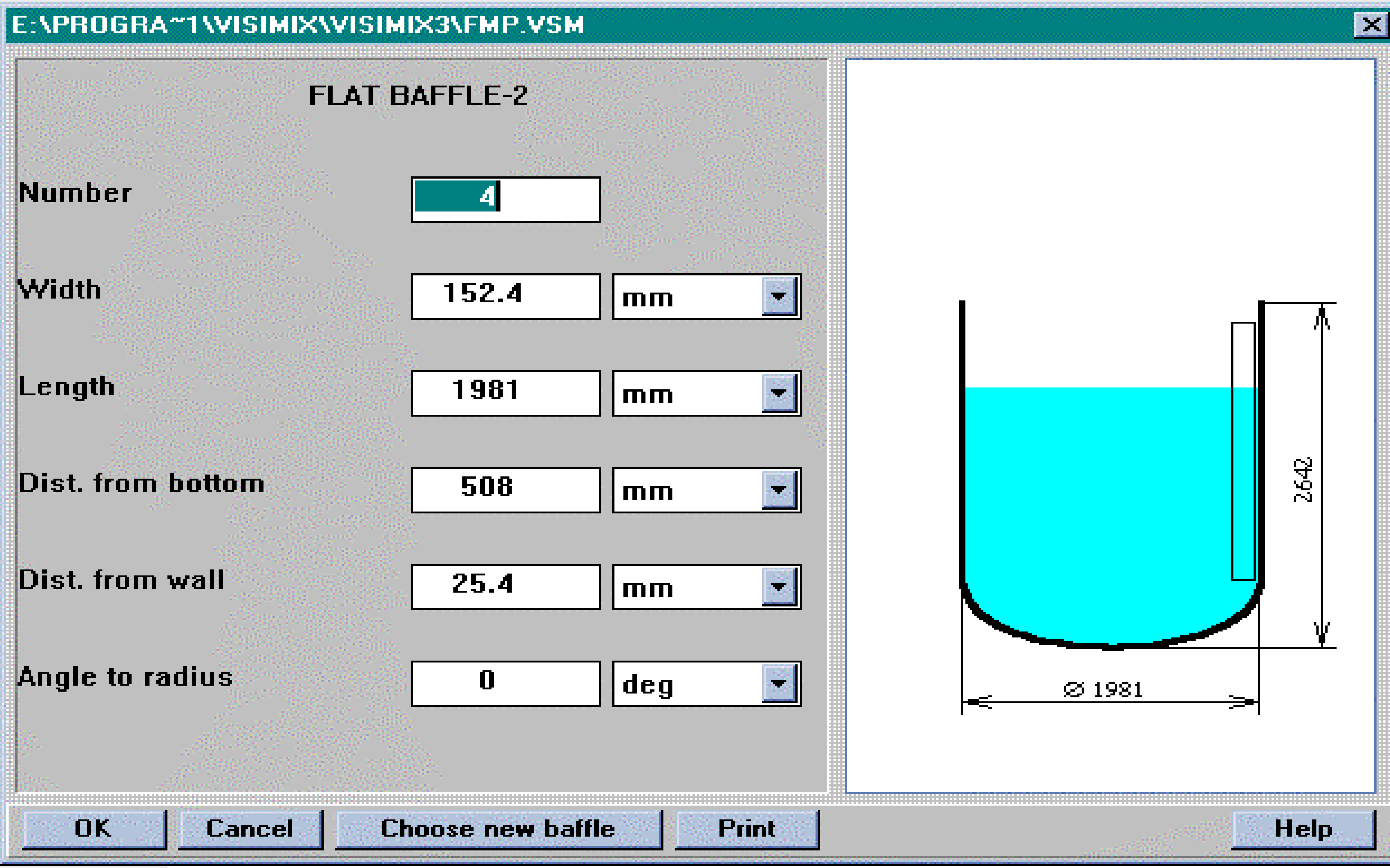

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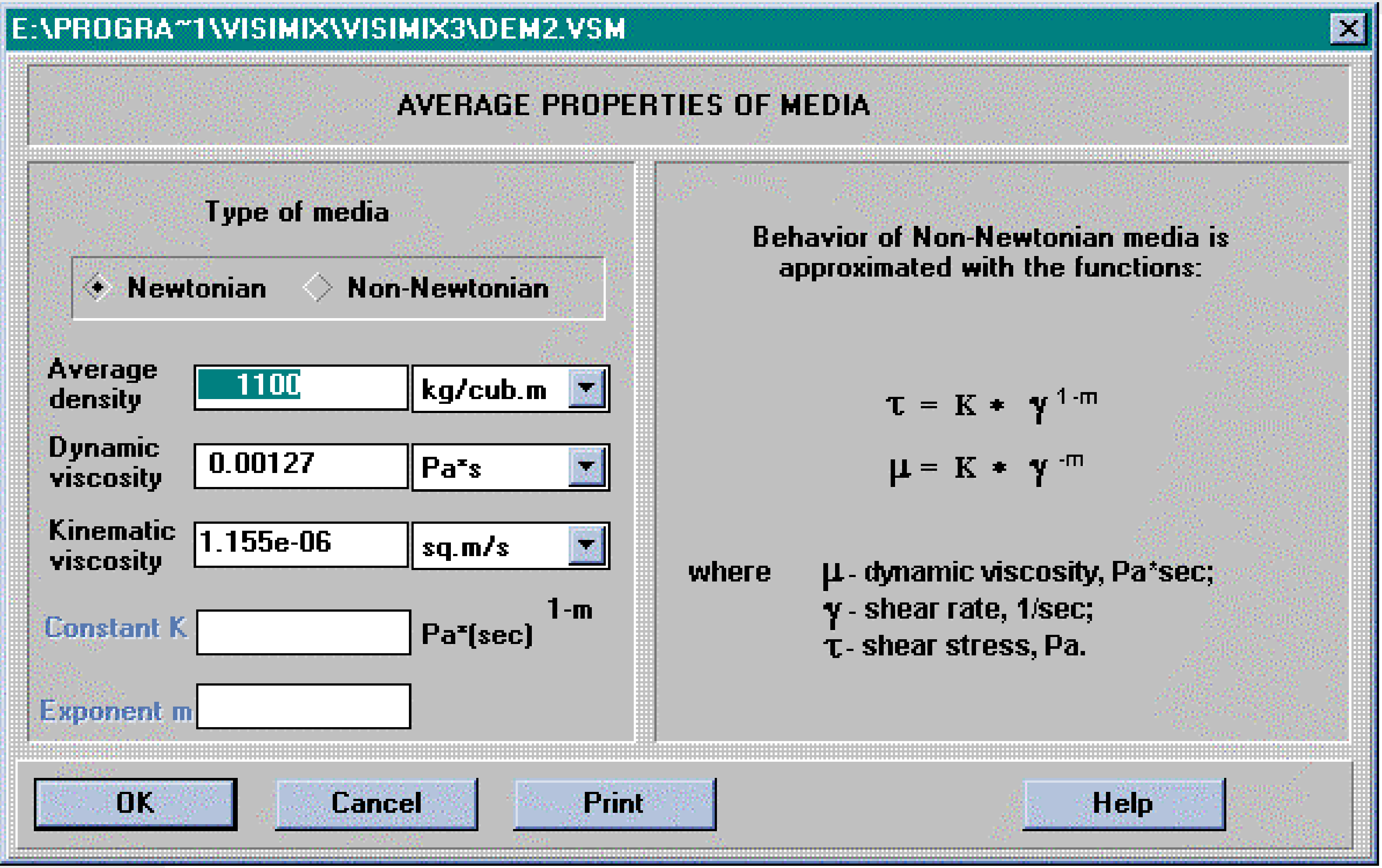

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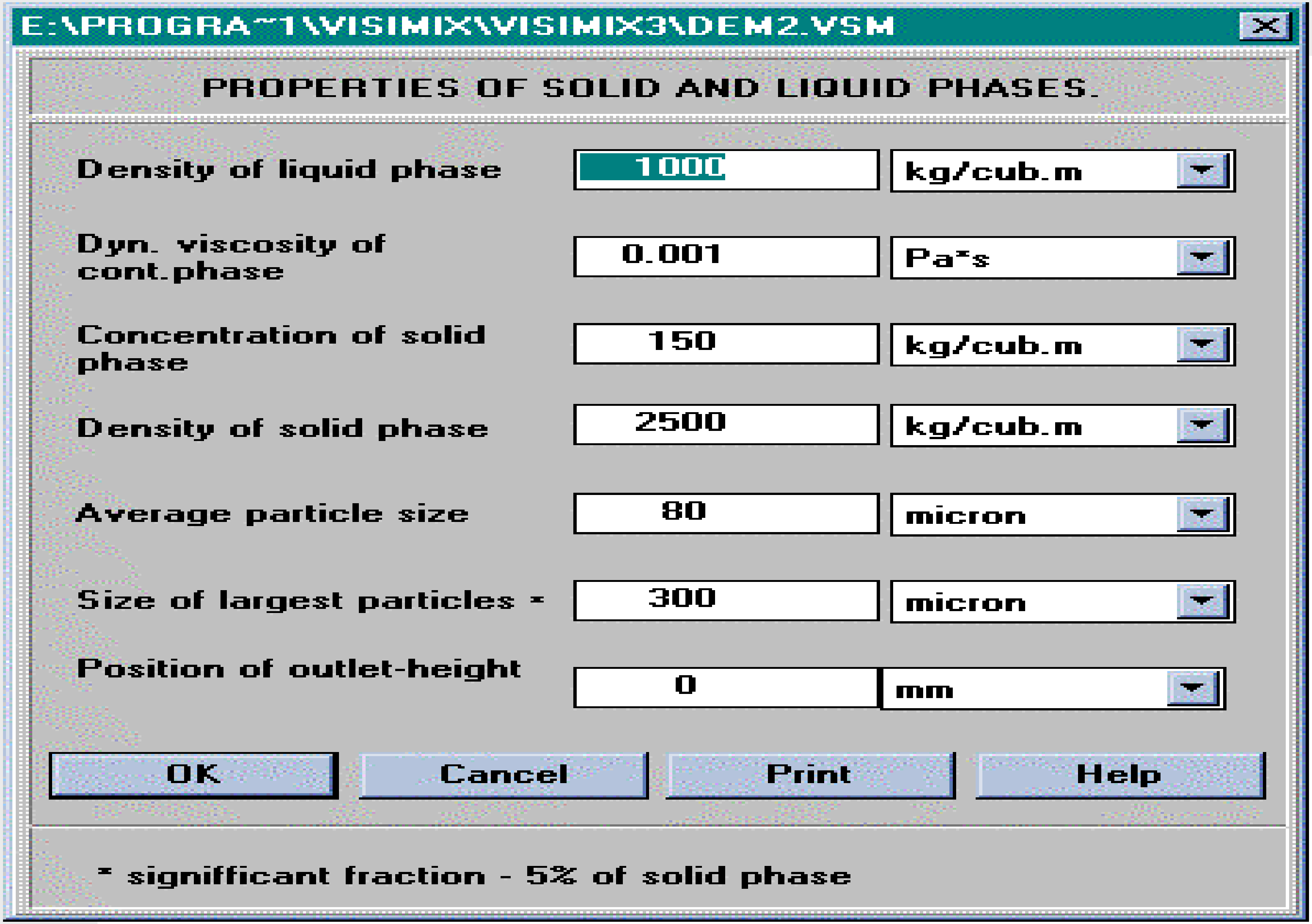

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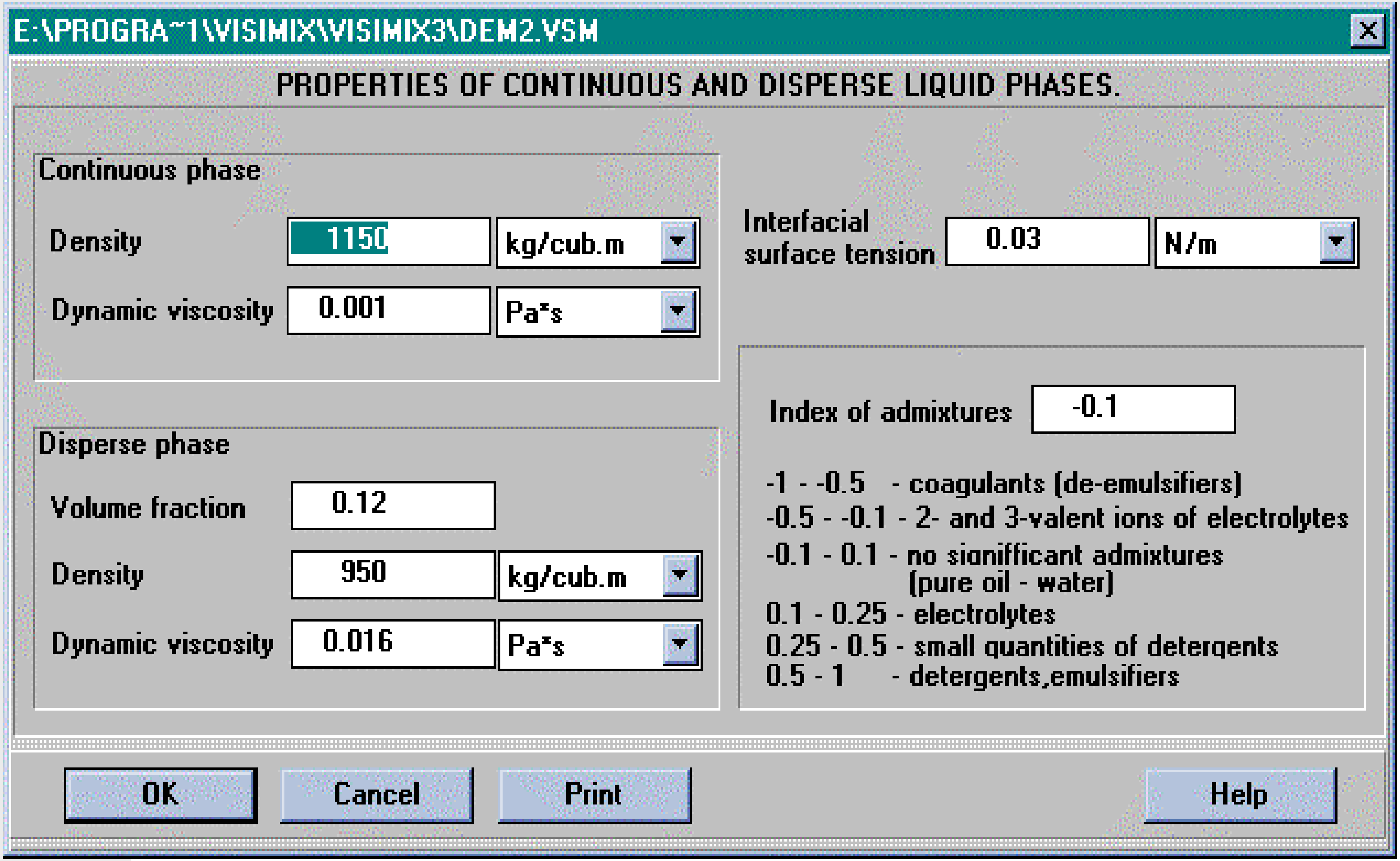

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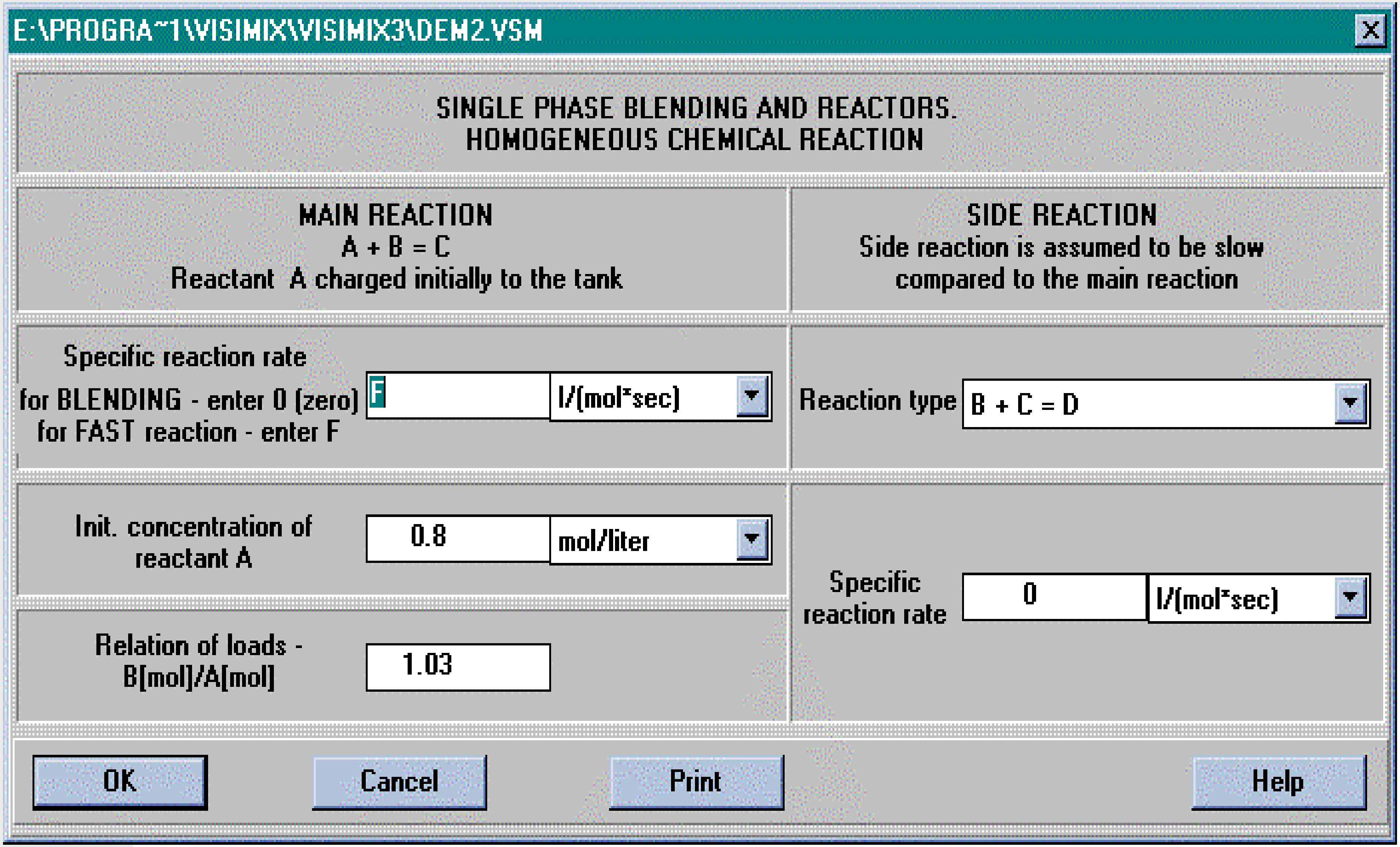


ACCESSIBILITY OF

VisiMix

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

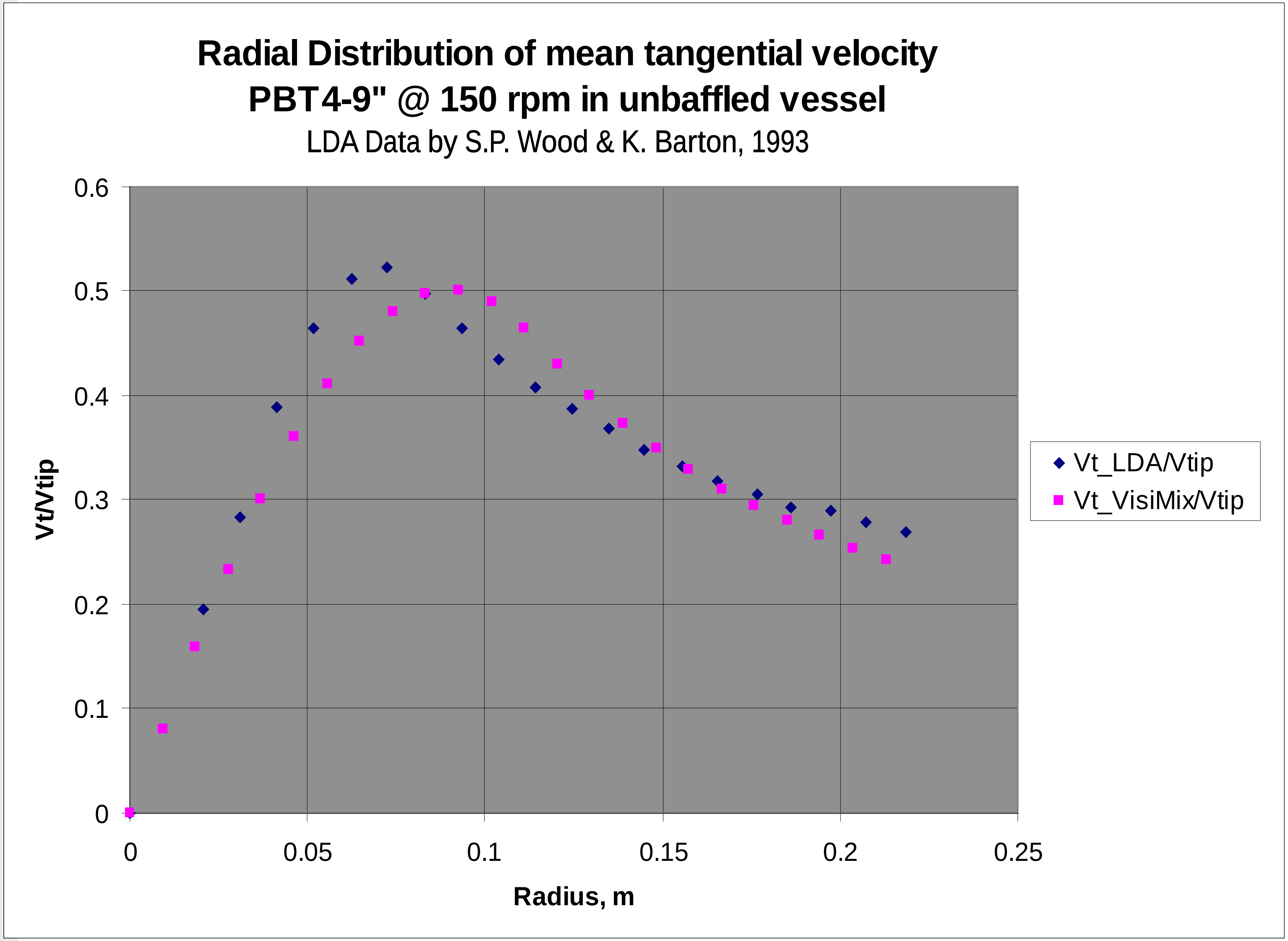
VisiMix

Reliability

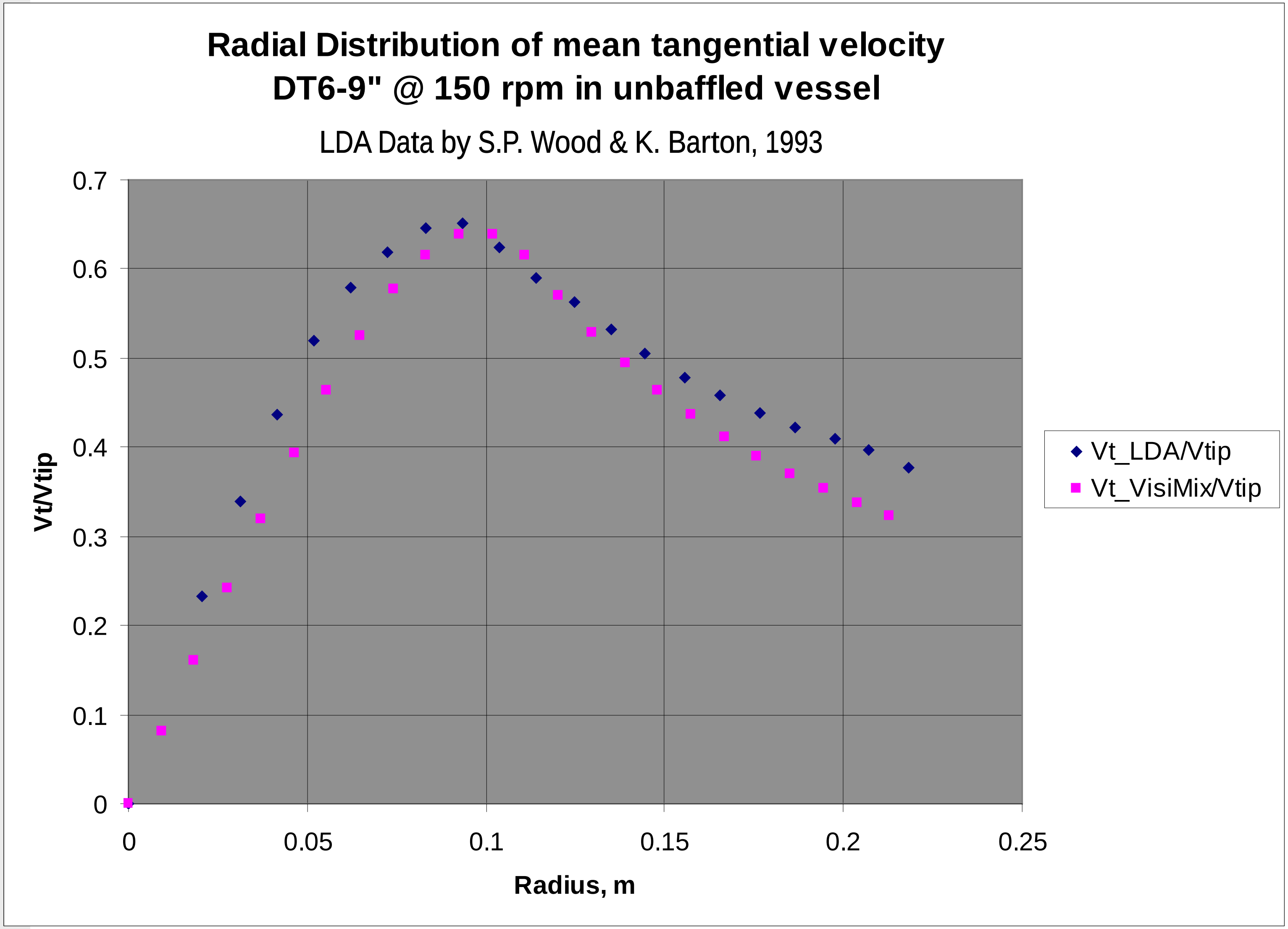
- Comparison with
  - data
  - established correlations

- Magnitude as well as functional dependence on key properties and parameters

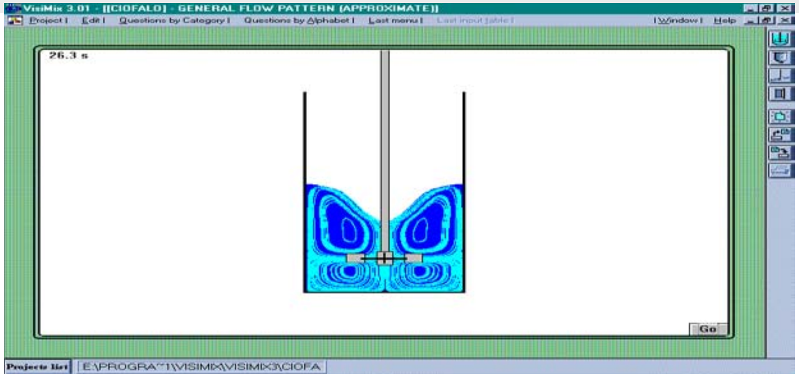
Reliability



Reliability



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

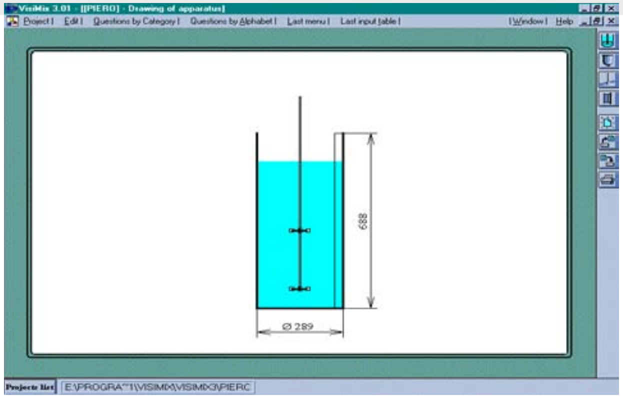
Reliability

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

	RDT	PBT	A310
Power Number, Po	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 d_{32} μm	VisiMix Results d_{32} μm	VisiMix Results 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

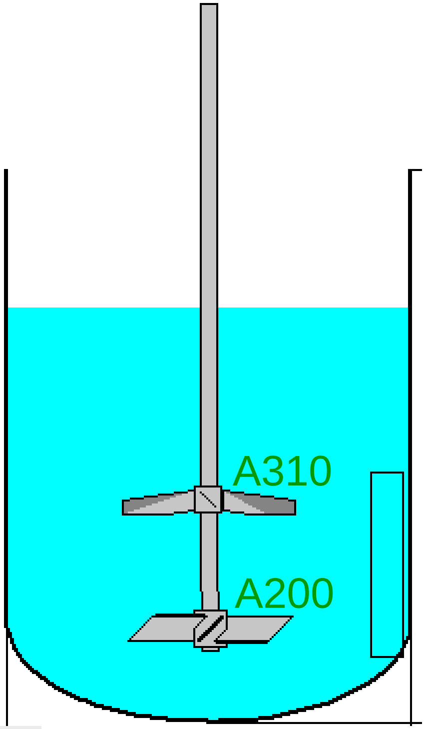
Reliability

- 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 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:

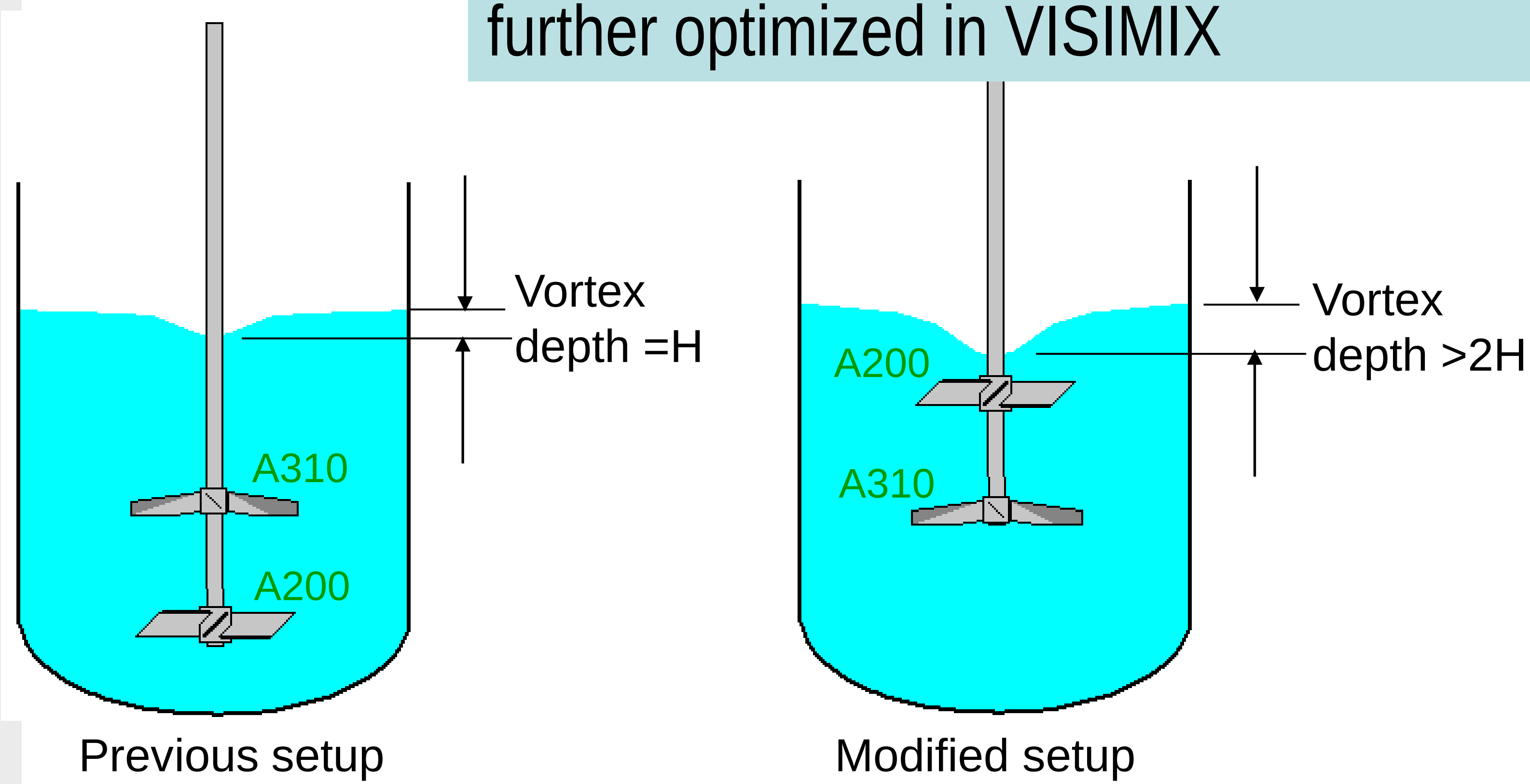
-- Impeller already operated at maximum rotation speed (RPM)

-- 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



-- 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

VisiMix 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!!)

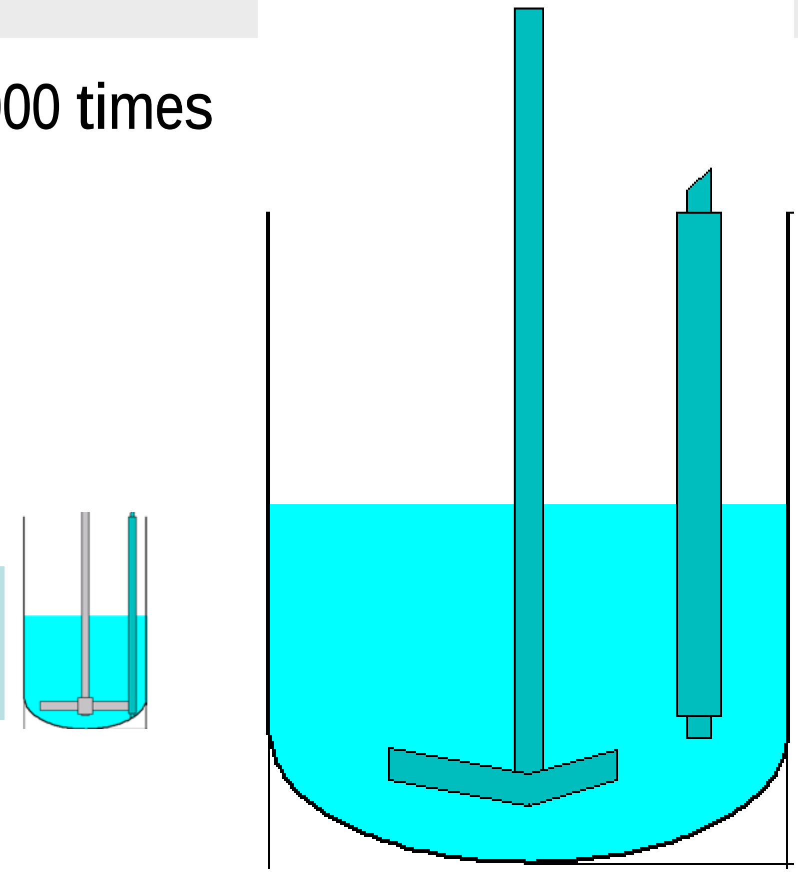
-- What reactor to choose?
choose from a few available/idle vessels & agitation systems to reduce capital

-- 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



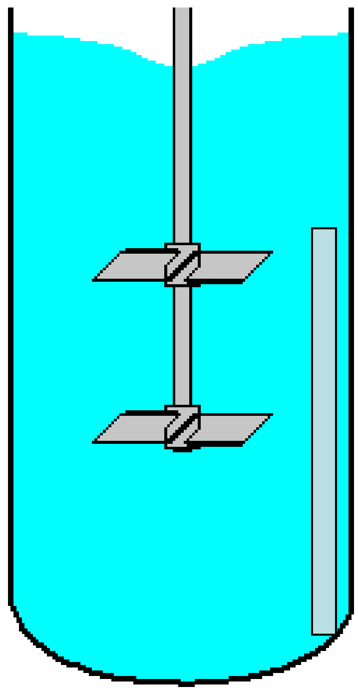
Lab Reactor:
Batch size: 700 cc
Batch weight: 0.6 kg

Commercial production Reactor:
Batch size: 7 m^3
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 m^3
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)

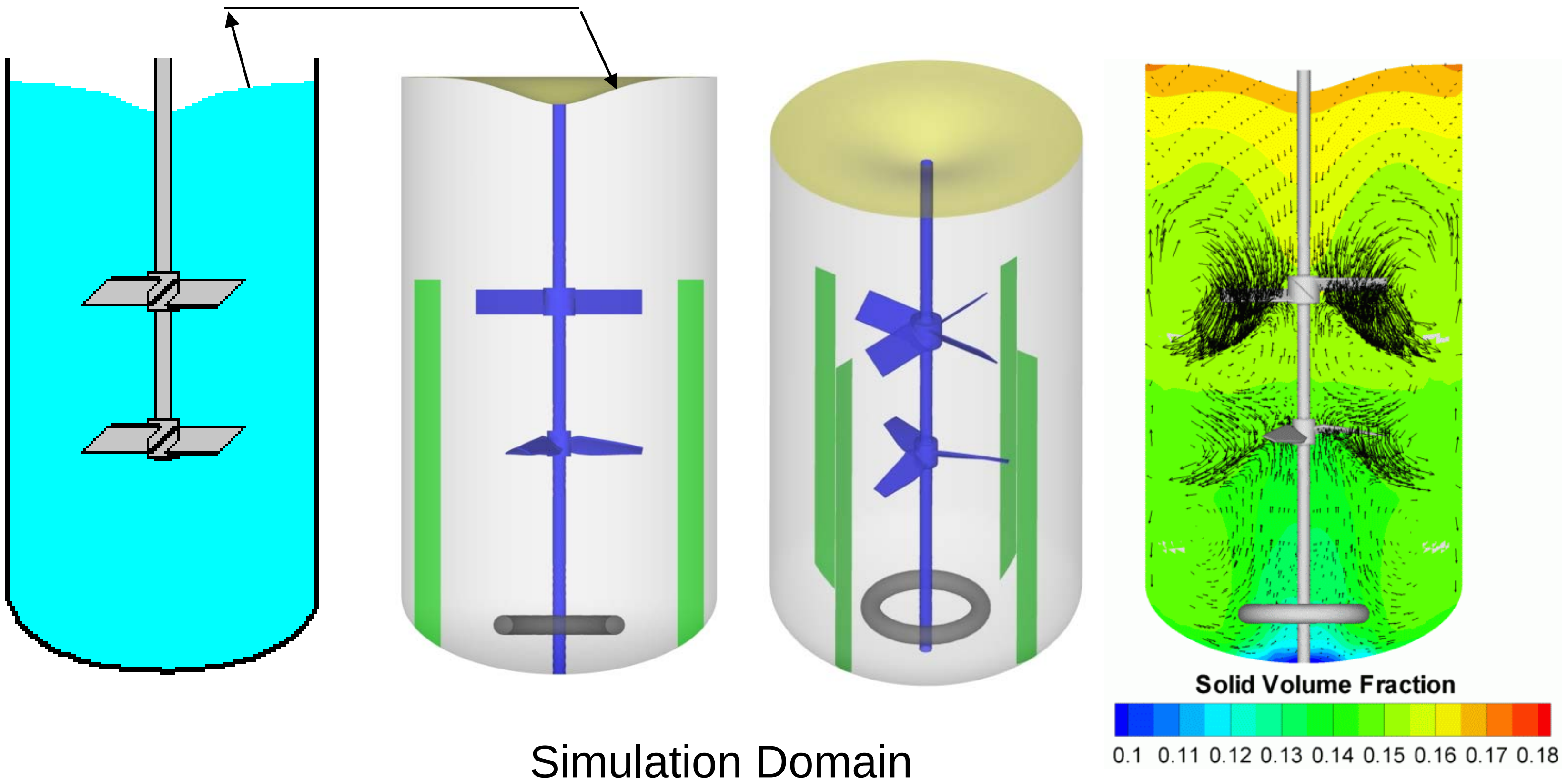
Use VISIMIX to predict the free surface (surface vortex)
Export the free surface geometry into CFD which is used as the domain top boundary specified with “slippery-wall” condition

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



Simulation Domain

VisiMix Application Case #4

comparing VISIMIX and lab experiments

Laboratory system to measure axial distribution of heavy solids

<u>chemical system</u>

40 wt% solids in NaCl

60 wt% salt tap water

2 g NaCl / kg tap water

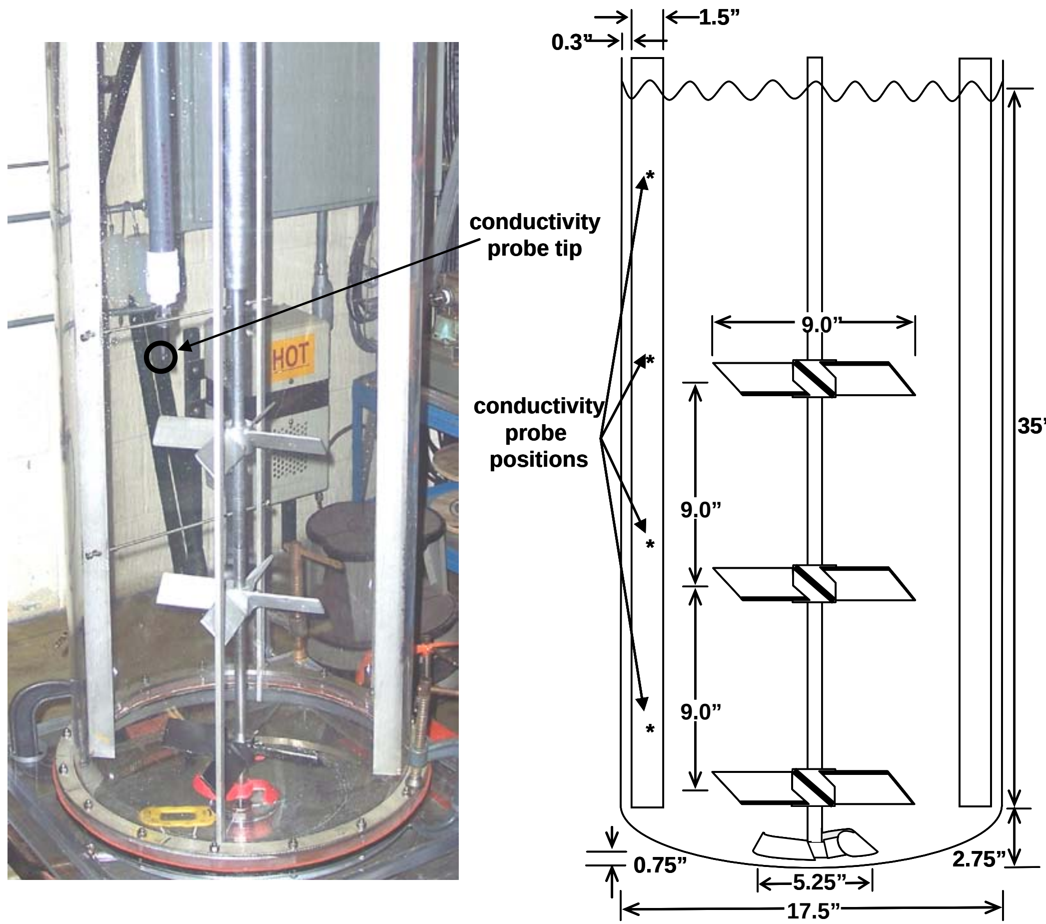
<u>Property of solid spheres</u>

ρ_{app} = 1.7 g/cc

d_p = 285 μm vol. med.

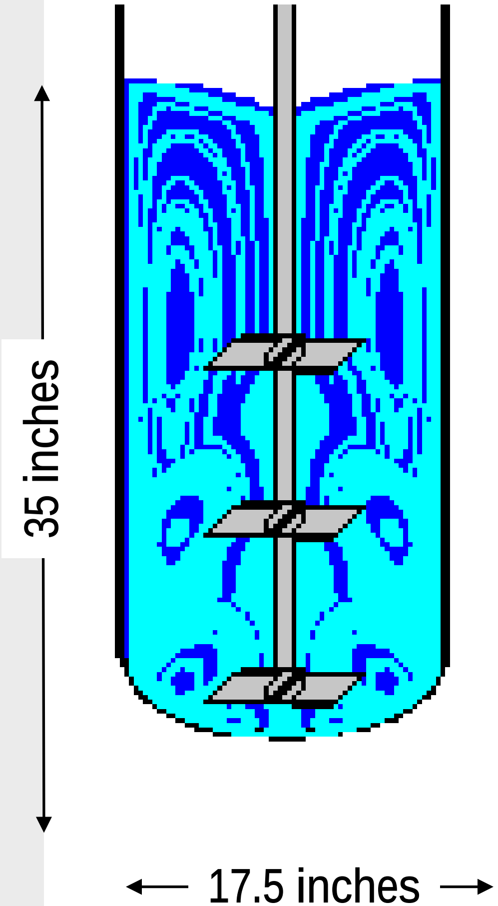
(<1 wt% 15-100 μm)

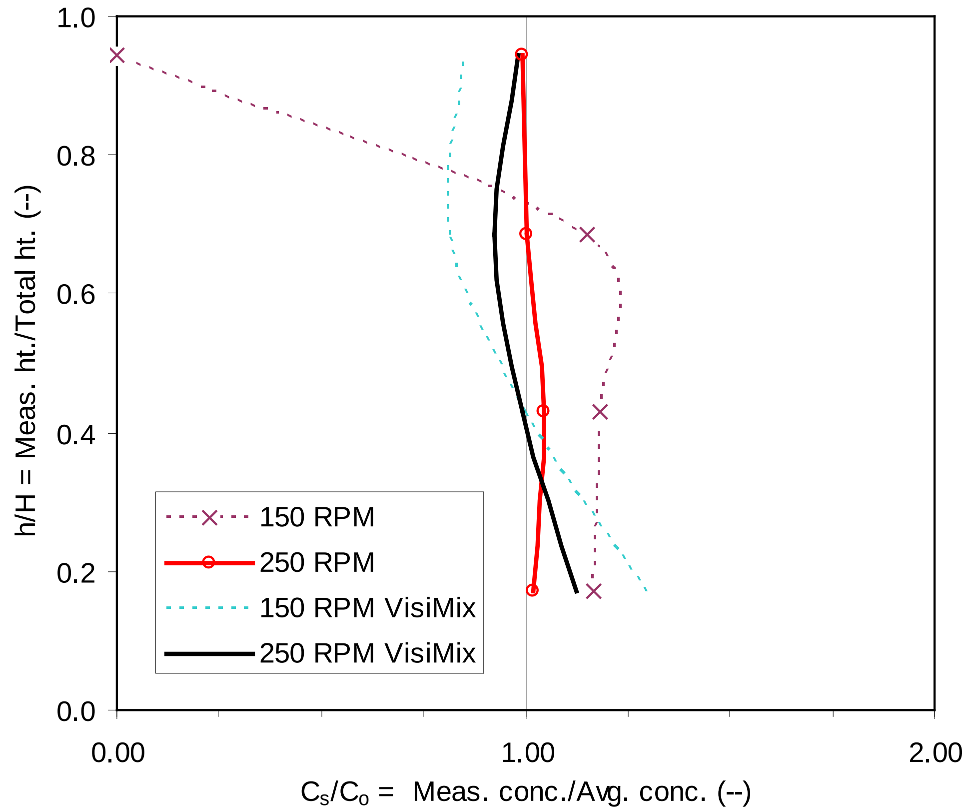
(<1.5 wt% 425-600 μm).



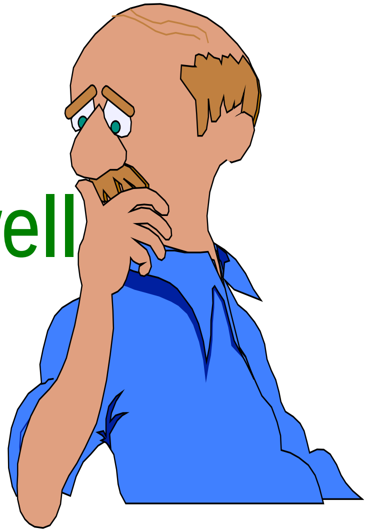
Normalized, axial solids distribution VisiMix vs. measured

Simulation: three standard PBTs





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
- Limited to included equipment geometries
- Limits of applicability not well defined